

Author Search

=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 14:32:59 ON 04 MAR 2008
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FILE COVERS 1907 - 4 Mar 2008 VOL 148 ISS 10
FILE LAST UPDATED: 3 Mar 2008 (20080303/ED)

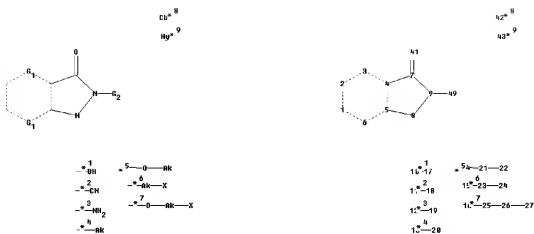
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> D QUE L40
L13 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading strB.str



G1:N,CH2,CH, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

G2:[*8], [*9]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
 19:CLASS 20:CLASS
 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 41:CLASS
 42:Atom 43:Atom
 49:CLASS

Generic attributes :

42:

Saturation : Unsaturated

Type of Ring System : Monocyclic

Element Count :
Node 20: Limited
C,C1-4

Node 22: Limited
C,C1-4

Node 23: Limited
C,C1-4

Node 26: Limited
C,C1-4

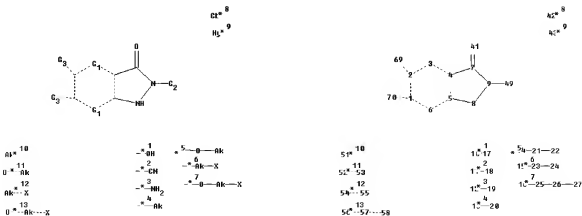
Node 42: Limited
C,C6

Node 43: Limited
N,N1-3

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L16      660 SEA FILE=REGISTRY SSS FUL L13
L31      STR
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading strE.str



```
chain nodes :
10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 41 42 43
49 51 52 53 54 55 56 57 58 69 70
ring nodes :
```

```

1 2 3 4 5 6 7 8 9
chain bonds :
1-70 2-69 7-41 9-49 10-17 11-18 12-19 13-20 14-21 15-23 16-25 21-22 23-
24
25-26 26-27 52-53 54-55 56-57 57-58
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-8 7-9 8-9
exact/norm bonds :
1-2 1-6 1-70 2-3 2-69 3-4 4-5 4-7 5-6 5-8 7-9 7-41 8-9 9-49 10-17
11-18 12-19 13-20 14-21 15-23 16-25 21-22 23-24 25-26 26-27 52-53 54-55
56-57 57-58
isolated ring systems :
containing 1 :

```

G1:N,CH2,CH, [*1], [*2], [*3], [*4], [*5], [*6], [*7]

G2:[*8], [*9]

G3:H,OH,CN,N,X, [*8], [*9], [*10], [*11], [*12], [*13]

Connectivity :

```

20:1 E exact RC ring/chain 22:1 E exact RC ring/chain 23:2 E exact RC ring/chain
26:2 E exact RC ring/chain 51:1 E exact RC ring/chain 53:1 E exact RC ring/chain
54:2 E exact
RC ring/chain 57:2 E exact RC ring/chain

```

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 41:CLASS
42:Atom 43:Atom
49:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS
58:CLASS 69:CLASS
70:CLASS

```

Generic attributes :

```

42:
Saturation          : Unsaturated
Type of Ring System : Monocyclic

```

Element Count :

Node 20: Limited
C,C1-4

Node 22: Limited
C,C1-4

Node 23: Limited
C,C1-4

Node 26: Limited
C,C1-4

Node 42: Limited
C,C6

Node 43: Limited
N,N1-3

Node 51: Limited

C,C1-4

Node 53: Limited
C,C1-4Node 54: Limited
C,C1-4Node 57: Limited
C,C1-4

L34 248 SEA FILE=REGISTRY SUB=L16 SSS FUL L31
 L36 144 SEA FILE=HCAPLUS ABB=ON PLU=ON L34
 L37 133 SEA FILE=HCAPLUS ABB=ON PLU=ON L36 AND (PRY<=2003 OR
 AY<=2003 OR PY<=2003)
 L38 24 SEA FILE=HCAPLUS ABB=ON PLU=ON BURKAMP F?/AU
 L39 405 SEA FILE=HCAPLUS ABB=ON PLU=ON FLETCHER S?/AU
 L40 1 SEA FILE=HCAPLUS ABB=ON PLU=ON (L38 OR L39) AND L37

=> D IBIB ED ABS FHITSTR L40 1

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS ON STN
 ACCESSION NUMBER: 2005:472147 HCAPLUS Full-text
 DOCUMENT NUMBER: 143:26598
 TITLE: Indazol-3-ones and analogs and derivatives which
 modulate the function of the vanilloid-1 receptor
 (VR1)
 INVENTOR(S): Burkamp, Frank; Fletcher, Stephen
 Robert
 PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|--------------|
| WO 2005049601 | A1 | 20050602 | WO 2004-GB4809 | 20041112 <-- |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| AU 2004290624 | A1 | 20050602 | AU 2004-290624 | 20041112 <-- |
| CA 2545710 | A1 | 20050602 | CA 2004-2545710 | 20041112 <-- |
| EP 1687293 | A1 | 20060809 | EP 2004-798529 | 20041112 <-- |
| EP 1687293 | B1 | 20070926 | | |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | |

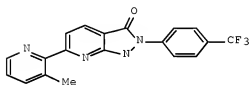
Serial No.:10/579,355

| | | | |
|------------------------|--|----------|-------------------------------|
| | IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS | | |
| CN 1882564 | A | 20061220 | CN 2004-80033693 20041112 <-- |
| JP 2007511495 | T | 20070510 | JP 2006-538958 20041112 <-- |
| AT 374195 | T | 20071015 | AT 2004-798529 20041112 <-- |
| US 2007129374 | A1 | 20070607 | US 2006-579355 20060511 <-- |
| IN 2006DN02932 | A | 20070803 | IN 2006-DN2932 20060522 <-- |
| PRIORITY APPLN. INFO.: | | | GB 2003-26633 A 20031114 <-- |
| | | | WO 2004-GB4809 W 20041112 |

OTHER SOURCE(S): CASREACT 143:26598; MARPAT 143:26598

ED Entered STN: 03 Jun 2005

GI



I

AB The title compds., which are useful as therapeutic compds., particularly in the treatment of pain and other conditions ameliorated by the modulation of the function of the vanilloid-1 receptor (VR1) are prepared E.g. I was prepared In vitro activity of I and similar compds. was determined in CHO cells, stably expressing recombinant human VR1 receptors. Increases in intracellular Ca²⁺ occurring after addition of test compound alone, prior to addition of capsaicin, allow determination of intrinsic agonist or partial agonist activity.

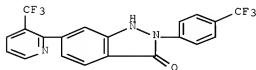
IT 852620-72-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indazol-3-ones for treatment of pain, inflammation and physiol. disorders ameliorated by the modulation of the function of the vanilloid-1 receptor (VR1))

RN 852620-72-5 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-[4-(trifluoromethyl)phenyl]-6-[3-(trifluoromethyl)-2-pyridinyl]- (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Structure Search

=> D QUE L37

L13 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L16 660 SEA FILE=REGISTRY SSS FUL L13

L31 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L34 248 SEA FILE=REGISTRY SUB=L16 SSS FUL L31

L36 144 SEA FILE=HCAPLUS ABB=ON PLU=ON L34

L37 133 SEA FILE=HCAPLUS ABB=ON PLU=ON L36 AND (PRY<=2003 OR
AY<=2003 OR PY<=2003)

=> S L37 NOT L40

L41 132 L37 NOT L40

=> D IBIB ED ABS HITSTR L41 1-15; D IBIB ED ABS HITSTR L41 60-75; D IBIB ED ABS
HITSTR L117-L133 L41

L41 ANSWER 1 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:981361 HCAPLUS Full-text

DOCUMENT NUMBER: 142:198064

TITLE: Process for preparation of 3-chloro-2-(4-chloro-2-
fluoro-5-hydroxyphenyl)-4,5,6,7-tetrahydro-2H-indazole
Jun, Dong Ju; Kim, Hyeong Rae; Park, Gwan Yong; Song,
Jong Hwan; Yoo, Eung GeolPATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.
KoreaSOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7

DOCUMENT TYPE: Patent

LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|--------------|
| ----- | ---- | ----- | ----- | ----- |
| KR 2003095677 | A | 20031224 | KR 2002-33207 | 20020614 <-- |
| PRIORITY APPLN. INFO.: | | | KR 2002-33207 | 20020614 <-- |

ED Entered STN: 17 Nov 2004

AB A process for preparing 3-chloro-2-(4-chloro-2-fluoro-5-hydroxyphenyl)-4,5,6,7-tetrahydro-2H-indazole is provided, thereby improving its preparation yield and converting byproducts of the preparation into starting material. A process for preparing 3-chloro-2-(4-chloro-2-fluoro-5-hydroxyphenyl)-4,5,6,7-tetrahydro-2H-indazole of the formula 1 comprises the steps of: reacting 2-(2-fluoro-4-chloro-5-hydroxyphenyl)-2,3a,4,5,6,7-hexahydroindazole-3-one of the formula 2 with phosgene; concentrating the phosgene reaction mixture under reduced pressure; dissolving the concentrate in an organic solvent; adding ammonia water or hydroxide solution to the organic solvent and filtering solids; and distilling the filtered solution, wherein the organic solvent is Et acetate; the addition of ammonia water or hydroxide solution is carried out at room temperature; the solids are mainly constituted of a compound of the

formula 2, and the byproducts of the reaction include a dimer represented by the formula 3a, 3b or 3c.

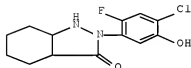
IT 122855-12-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of chloro(chlorofluorohydroxyphenyl)tetrahydroindazole)

RN 122855-12-3 HCAPLUS

CN 3H-Indazol-3-one, 2-(4-chloro-2-fluoro-5-hydroxyphenyl)octahydro- (CA INDEX NAME)



L41 ANSWER 2 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:333718 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:339518

TITLE: Preparation of morphinan derivatives having nitrogen-containing heterocyclic group as remedies or prophylactic agents for urinary frequency or urinary incontinence

INVENTOR(S): Izumimoto, Naoki; Kawai, Koji; Kawamura, Kuniaki; Fujimura, Morihiro; Komagata, Toshikazu

PATENT ASSIGNEE(S): Toray Industries, Inc., Japan

SOURCE: PCT Int. Appl., 202 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

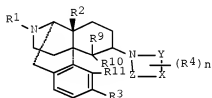
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----------------|--|----------|------------------|--------------|
| WO 2004033457 | A1 | 20040422 | WO 2003-JP12890 | 20031008 <-- |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| CA 2501389 | A1 | 20040422 | CA 2003-2501389 | 20031008 <-- |
| AU 2003272944 | A1 | 20040504 | AU 2003-272944 | 20031008 <-- |
| EP 1555266 | A1 | 20050720 | EP 2003-754030 | 20031008 <-- |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | |
| BR 2003014754 | A | 20050726 | BR 2003-14754 | 20031008 <-- |
| CN 1703415 | A | 20051130 | CN 2003-80100971 | 20031008 <-- |
| JP 4016986 | B2 | 20071205 | JP 2004-542845 | 20031008 <-- |
| IN 2005KN00466 | A | 20070105 | IN 2005-KN466 | 20050321 <-- |
| ZA 2005002650 | A | 20060628 | ZA 2005-2650 | 20050401 <-- |

Serial No.:10/579,355

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|------------------------|----|----------|-----------------|-----------------|
| US 2006040970 | A1 | 20060223 | US 2005-530664 | 20050406 <-- |
| US 7320984 | B2 | 20080122 | | |
| MX 2005PA03723 | A | 20050930 | MX 2005-PA3723 | 20050407 <-- |
| NO 2005002167 | A | 20050616 | NO 2005-2167 | 20050503 <-- |
| JP 2007224039 | A | 20070906 | JP 2007-106935 | 20070416 <-- |
| JP 2008044938 | A | 20080228 | JP 2007-195352 | 20070727 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2002-295616 | A 20021009 <-- |
| | | | JP 2004-542845 | A3 20031008 <-- |
| | | | WO 2003-JP12890 | W 20031008 <-- |

OTHER SOURCE(S): MARPAT 140:339518
 ED Entered STN: 23 Apr 2004
 GI



AB Title compds. I [wherein R1 represents Me, cyclopropylmethyl, etc.; R2 and R3 represent each hydroxy, methoxy, acetoxy, etc.; Y and Z represent each a valence bond, CO, etc.; X represents a C2-5 carbon chain constituting a part of the cyclic structure (wherein one of the carbon atoms may be substituted by oxygen, sulfur or nitrogen); (R4)n represents an optionally substituted fused benzene ring, carbonyl, etc.; R9 represents hydrogen, etc.; R10 and R11 may be bonded together to form O; and R6 represents hydrogen, etc.] and their pharmacol. acceptable salts, useful as remedy or a prophylactic agents for urinary frequency or urinary incontinence, are prepared Thus, refluxing dihydrocodeinone with 1,2,3,4-tetrahydroquinoline in xylene-DMF in the presence of methanesulfonic acid gave, after treatment with sodium cyanohydride and methanesulfonic acid in methanol at room temperature for 24 h, 33% 4,5a-epoxy-6β-tetrahydroquinolino-3- methoxy-17-methylmorphinan (II). II was converted to 4,5a-epoxy- 6β-tetrahydroquinolino-17-methylmorphinan-3-ol tartrate (III) in 75% yield. III showed urinary contraction inhibitory activity at 0.1 mg/kg i.v. in rats.

IT 681032-41-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of morphinan derivs. having nitrogen-containing heterocyclic group as remedies or prophylactic agents for urinary frequency or urinary incontinence)

RN 681032-41-7 HCAPLUS

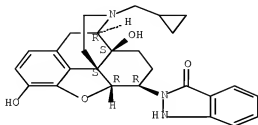
CN 3H-Indazol-3-one, 2-[(5a,6β)-17-(cyclopropylmethyl)-4,5-epoxy-3,14-dihydroxymorphinan-6-yl]-1,2-dihydro-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 681032-40-6

CMF C27 H29 N3 O4

Absolute stereochemistry.

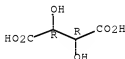


CM 2

CRN 87-69-4

CMF C4 H6 O6

Absolute stereochemistry.



IT 681032-40-6P

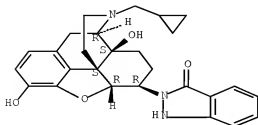
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)

(preparation of morphinan derivs. having nitrogen-containing heterocyclic
group as remedies or prophylactic agents for urinary frequency or urinary
incontinence)

RN 681032-40-6 HCAPLUS

CN 3H-Indazol-3-one, 2-[(5 α ,6 β)-17-(cyclopropylmethyl)-4,5-epoxy-
3,14-dihydroxymorphinan-6-yl]-1,2-dihydro- (9CI) (CA INDEX NAME)

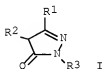
Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 3 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:777767 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 139:286349
 TITLE: Medicine for prevention and/or therapy of cardiomyopathy
 INVENTOR(S): Hayashi, Tetsuya
 PATENT ASSIGNEE(S): Mitsubishi Pharma Corporation, Japan
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------------|
| ----- | ---- | ----- | ----- | ----- |
| WO 2003080583 | A1 | 20031002 | WO 2003-JP3813 | 20030327 <-- |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| AU 2003227257 | A1 | 20031008 | AU 2003-227257 | 20030327 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2002-87499 | A 20020327 <-- |
| | | | WO 2003-JP3813 | W 20030327 <-- |
| OTHER SOURCE(S): | MARPAT 139:286349 | | | |
| ED Entered STN: | 03 Oct 2003 | | | |
| GI | | | | |



AB A medicine for prevention and/or therapy of cardiomyopathy, which comprises, as an active constituent, a pyrazolone derivative represented by the following formula I (R1 = H, aryl, alkyl or alkoxy carbonyl-alkyl group, and R2 = H, aryloxy, aryl-mercapto, alkyl or hydroxyalkyl group, or R1, R2 = alkylene group, and R3 = H, alkyl, cycloalkyl, hydroxyalkyl, benzyl, naphthyl, Ph group, or a Ph group substituted with the same or different one to three substituents selected from the group consisting of alkyl, alkoxy, hydroxyalkyl, alkoxy carbonyl, alkyl-mercapto, alkylamino, dialkylamino,

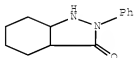
halogen atom, trifluoromethyl, carboxyl, cyano, hydroxyl, nitro, amino and acetamido group), or a pharmaceutically acceptable salt thereof.

IT 70972-70-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(medicine for prevention and/or therapy of cardiomyopathy)

RN 70972-70-2 HCAPLUS

CN 3H-Indazol-3-one, octahydro-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 4 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003/757683 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:261293

TITLE: Preventive and/or therapeutic agent for hypoxic ischemic brain disorder

INVENTOR(S): Ikeda, Tomoaki; Ikenoue, Tsuyomu

PATENT ASSIGNEE(S): Mitsubishi Pharma Corporation, Japan

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------------|
| WO 2003078401 | A1 | 20030925 | WO 2003-JP3067 | 20030314 <-- |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| JP 2005343789 | A | 20051215 | JP 2002-71595 | 20020315 <-- |
| AU 2003213364 | A1 | 20030929 | AU 2003-213364 | 20030314 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2002-71595 | A 20020315 <-- |
| | | | WO 2003-JP3067 | W 20030314 <-- |

OTHER SOURCE(S): MARPAT 139:261293

ED Entered STN: 26 Sep 2003

AB The patent relates to a medicine for use in the prevention of and/or treatments for hypoxic ischemic brain disorders, especially ones of newborns caused by labor. It contains as an active ingredient a substance selected from the group consisting of 3-methyl-1-phenyl-2-pyrazolin-5-one, pyrazolozone derivs. which are analogs thereof, physiol. acceptable salts thereof, and any hydrates and any solvates of these. Thus, 1-phenyl-3-methyl-2-pyrazolin-5-one

prepared by refluxing Et acetoacetate with phenylhydrazine in ethanol and recrystn. was dissolved in simulated body fluid and showed effect on hypoxic ischemic brain of new born rat.

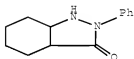
IT 70972-70-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pyrazolinone derivative for preventive and/or therapeutic agent for hypoxic ischemic brain disorder)

RN 70972-70-2 HCAPLUS

CN 3H-Indazol-3-one, octahydro-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 5 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:868631 HCAPLUS Full-text

DOCUMENT NUMBER: 138:137685

TITLE: Preliminary study of the non-emissive thermal rearrangement of novel N-cyanates to rigid rod polymers

AUTHOR(S): Hay, John N.; Martin, Philip S.; Bird, Clive W.; Hormozi, Neda

CORPORATE SOURCE: Department of Chemistry, University of Surrey, Surrey, GU2 7XH, UK

SOURCE: Polymer International (2002), 51(10), 1031-1036

CODEN: PLYIEI; ISSN: 0959-8103

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 15 Nov 2002

AB Novel materials, both monomeric and polymeric, were synthesized to study the non-emissive thermal rearrangement of N-cyanates. These materials undergo an exothermic rearrangement, at temps. in the range of 150-300°, to fused heterocyclic products. The series of N-cyanate polymeric materials was characterized by FTIR and modulated DSC as a preliminary assessment of their use as processable precursors to rigid rod polymers.

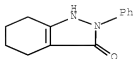
IT 62221-94-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(non-emissive thermal rearrangement of N-cyanates to rigid rod polymers)

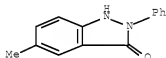
RN 62221-94-7 HCAPLUS

CN 3H-Indazol-3-one, 1,2,4,5,6,7-hexahydro-2-phenyl- (CA INDEX NAME)

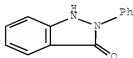


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 6 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:855866 HCAPLUS Full-text
 DOCUMENT NUMBER: 139:214345
 TITLE: Product class 2: 1H- and 2H-indazoles
 AUTHOR(S): Stadlbauer, W.
 CORPORATE SOURCE: Institut für Organische Chemie, Karl-Franzens-Universität, Graz, A-8010, Austria
 SOURCE: Science of Synthesis (2002), 12, 227-324
 CODEN: SSCYJ9
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English
 ED Entered STN: 12 Nov 2002
 AB A review of methods for preparation of 1H- and 2H-indazoles. Covered reactions include ring-closure reactions, ring transformations, and substituent modifications.
 IT 17049-62-6P 17049-65-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of 1H- and 2H-indazoles via ring-closure reactions, ring transformations, and substituent modifications)
 RN 17049-62-6 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-5-methyl-2-phenyl- (CA INDEX NAME)



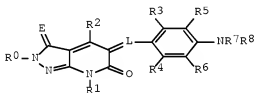
RN 17049-65-9 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 664 THERE ARE 664 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

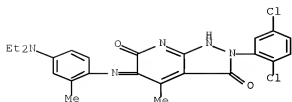
L41 ANSWER 7 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:447150 HCAPLUS Full-text
 DOCUMENT NUMBER: 137:39273
 TITLE: Silver halide color print material containing solid dye dispersions for motion picture
 INVENTOR(S): Tanemura, Hatsumi
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 70 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------|------|------------------|-----------------|--------------|
| JP 2002169254 | A | 20020614 | JP 2000-364911 | 20001130 <-- |
| PRIORITY APPLN. INFO.: | | | JP 2000-364911 | 20001130 <-- |
| OTHER SOURCE(S): | | MARPAT 137:39273 | | |
| ED Entered STN: 14 Jun 2002 | | | | |
| GI | | | | |



I

- AB The material comprises nonphotosensitive hydrophilic colloid layer(s) and ≥ 1 blue-, green-, and red-sensitive emulsion layer on a transparent support, contg Ag halide grains with AgCl content ≥ 90 mol% and dispersion of solid dye I (L = N, group linked with 1, 3, 5, or 7 (substituted) methine through conjugated double bond; E = O, S, NR9; R0, R9 = H, alkyl, alkenyl, alkynyl, aryl, heterocycle, amino, hydrazino, diazenyl; R1 = H, alkyl, aryl, alkenyl, alkynyl, heterocycle; R2 = H, halo, CN, NO2, OH, CO2H, alkyl, aryl, alkenyl, heterocycle, alkoxy, aryloxy, alkoxycarbonyl, aryloxy, carbamoyl, sulfamoyl, alkylthio, arylthio, alkylsulfonfyl, arylsulfonfyl, alkynyl; R0 and R9 may form a ring; R3, R4 = H, halo, alkoxy, alkyl, alkenyl, aryloxy, aryl; R5, R6 = H, substituent; R7, R8 = alkyl, aryl, vinyl, acyl, alkyl- or aryl-sulfonfyl; R3 and R5, R4 and R6, R7 and R8, R5 and R7, and R6 and R8 may form a ring). It showed improved antihalation and handling properties under safelight, storage stability, sharpness, and high speed processing properties.
- IT 137079-55-1P
 RL: PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (cinephotos. film containing dye solid dispersion)
- RN 137079-55-1 HCAPLUS
- CN 2H-Pyrazolo[3,4-b]pyridine-3,6(5H,7H)-dione, 2-(2,5-dichlorophenyl)-5-[[4-(diethylamino)-2-methylphenyl]imino]-4-methyl- (9CI) (CA INDEX NAME)

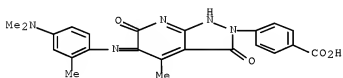


IT 163073-35-6

RL: TEM (Technical or engineered material use); USES (Uses)
(cinephoto. film containing dye solid dispersion)

RN 163073-35-6 HCAPLUS

CN Benzoic acid, 4-[5-[[4-(dimethylamino)-2-methylphenyl]imino]-1,3,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl]- (CA INDEX NAME)

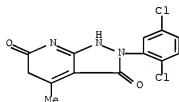


IT 137079-59-5P

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)
(preparation of dye)

RN 137079-59-5 HCAPLUS

CN 2H-Pyrazolo[3,4-b]pyridine-3,6(5H,7H)-dione, 2-(2,5-dichlorophenyl)-4-methyl- (9CI) (CA INDEX NAME)

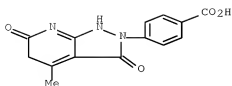


IT 190380-26-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dye)

RN 190380-26-8 HCAPLUS

CN Benzoic acid, 4-(1,3,5,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl)- (CA INDEX NAME)



L41 ANSWER 8 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:391720 HCAPLUS Full-text
 DOCUMENT NUMBER: 136:386144
 TITLE: Preparation of pyrrolo[2,1-f][1,2,4]triazine
 carboxylic acid derivatives for use in treating p38
 kinase-associated conditions
 INVENTOR(S): Leftheris, Katerina; Barrish, Joel; Hynes, John;
 Wroblewski, Stephen T.
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 108 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

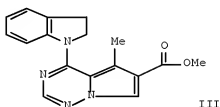
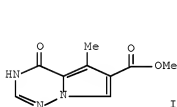
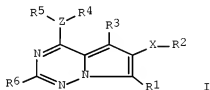
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 2002040486 | A2 | 20020523 | WO 2001-US49982 | 20011107 <-- |
| WO 2002040486 | A3 | 20030912 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2429628 | A1 | 20020523 | CA 2001-2429628 | 20011107 <-- |
| AU 2002032760 | A | 20020527 | AU 2002-32760 | 20011107 <-- |
| EE 200300227 | A | 20031015 | EE 2003-227 | 20011107 <-- |
| EP 1363910 | A2 | 20031126 | EP 2001-992298 | 20011107 <-- |
| EP 1363910 | B1 | 20060301 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| HU 2003003897 | A2 | 20040301 | HU 2003-3897 | 20011107 <-- |
| JP 2004522713 | T | 20040729 | JP 2002-543494 | 20011107 <-- |
| CN 1622946 | A | 20050601 | CN 2001-818997 | 20011107 <-- |
| NZ 525334 | A | 20050729 | NZ 2001-525334 | 20011107 <-- |
| BR 2001015446 | A | 20050809 | BR 2001-15446 | 20011107 <-- |
| AT 318820 | T | 20060315 | AT 2001-992298 | 20011107 <-- |
| PT 1363910 | T | 20060531 | PT 2001-992298 | 20011107 <-- |
| ES 2259051 | T3 | 20060916 | ES 2001-992298 | 20011107 <-- |
| RU 2316556 | C2 | 20080210 | RU 2003-117799 | 20011107 <-- |
| BG 107750 | A | 20040130 | BG 2003-107750 | 20030421 <-- |
| IN 2003MN00471 | A | 20050304 | IN 2003-MN471 | 20030502 <-- |

| | | | | |
|------------------------|----|----------|-----------------|----------------|
| MX 2003PA04290 | A | 20040212 | MX 2003-PA4290 | 20030515 <-- |
| ZA 2003003786 | A | 20040816 | ZA 2003-3786 | 20030515 <-- |
| NO 2003002229 | A | 20030716 | NO 2003-2229 | 20030516 <-- |
| HK 1057555 | A1 | 20060915 | HK 2004-100424 | 20040119 <-- |
| PRIORITY APPLN. INFO.: | | | US 2000-249877P | P 20001117 <-- |
| | | | US 2001-310561P | P 20010807 <-- |
| | | | WO 2001-US49982 | W 20011107 <-- |

OTHER SOURCE(S): MARPAT 136:386144

ED Entered STN: 24 May 2002

GI

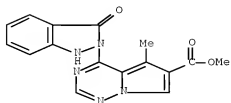


- AB Title compds. I [R3 = H, Me, perfluoromethyl, MeO, halo, cyano, NH2; X = O, OC(O), S, S(O), SO2, C(O), CO2, amino, aminoacyl, etc. or X is absent; Z = O, S, N, and CR20, wherein when Z = CR20 said carbon atom may form an (un)(un)substituted bicyclic aryl or heteroaryl with R4 and R5; R1 = H, CH3, OH, OCH3, SH, SCH3, acyloxy, etc.; R2 = H, alkyl, alkenyl, aryl, heteroaryl, etc.; R4 = (un)substituted aryl, heteroaryl, bicyclic 7-11 membered (un)saturated carbocyclic or heterocyclic ring; R5 = H, alkyl, etc. or alternatively, R4 and R5 taken together with Z form an (un)substituted bicyclic 7-11 membered aryl or heteroaryl; R6 = H, alkyl, aryl, heterocyclo, etc.; R20 = H, alkyl, etc. with some provisions] were prepared Over 150 compds. were disclosed. For instance, 1-Amino-3-methylpyrrole- 2,4-dicarboxylic acid di-Me ester was prepared from the parent pyrrole (preparation given) and diphenylphosphorylhydroxylamine and reacted with formamide (165°C, 6 h) to give intermediate pyrrolo[2,1-f][1,2,4]triazine II in 90% yield. II was converted to the imino-chloride (POC13) and treated with indoline to give example compound III. I are inhibitors of p38 kinase and are useful for the treatment of inflammatory disorders.
- IT 319#13-16-4P, 4-[2,3-Dihydro-3-oxo-1H-indazol-2-yl]-5-methylpyrrolo[2,1-f][1,2,4]triazine-6-carboxylic acid methyl ester
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug; preparation of pyrrolo[2,1-f][1,2,4]triazine carboxylic acid derivs.

for use in treating p38 kinase-associated conditions)

RN 310443-16-4 HCAPLUS

CN Pyrrolo[2,1-f][1,2,4]triazine-6-carboxylic acid, 4-(1,3-dihydro-3-oxo-2H-indazol-2-yl)-5-methyl-, methyl ester (CA INDEX NAME)



L41 ANSWER 9 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:633844 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:357894

TITLE:

Synthesis of new pyrazolo[1,5-a]pyrimidines and pyrazolo[3,4-b]pyridines

AUTHOR(S): Al-Mousawi, Saleh M.; Mohammad, Mohammad A.; Elnagdi, Mohamad H.

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Kuwait, Safat, 13060, Kuwait

SOURCE: Journal of Heterocyclic Chemistry (2001), 38(4), 989-991

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

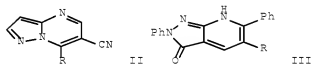
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:357894

ED Entered STN: 31 Aug 2001

GI



AB While 3(5)-aminopyrazole reacts with enamionitrile RR1C:CHNMe2 (I, R = cyano, R1 = PhCO, cyano) to yield pyrazolo[1,5-a]pyrimidines II, 3-amino-5-pyrazolone reacts with the same reagents, I (R = cyano, H, R1 = PhCO) to yield pyrazolo[3,4-b]pyridines III (R = cyano, H).

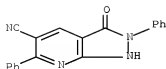
IT 3/3385-54-7P 3/3385-55-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

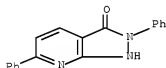
(preparation of pyrazolopyrimidines and pyrazolopyridines by cycloaddn. of pyrazoles with enamionones and enamionitriles)

RN 3/3385-54-7 HCAPLUS

CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 2,3-dihydro-3-oxo-2,6-diphenyl- (CA INDEX NAME)



RN 373385-55-8 HCAPLUS
 CN 3H-Pyrazolo[3,4-b]pyridin-3-one, 1,2-dihydro-2,6-diphenyl- (CA INDEX NAME)



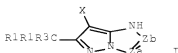
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 10 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:414657 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 135:26820
 TITLE: Silver halide color photographic material for movies
 INVENTOR(S): Sakai, Shuichi
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 68 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|--------------|
| JP 2001154318 | A | 20010608 | JP 1999-334982 | 19991125 <-- |
| CN 1298122 | A | 20010606 | CN 2000-132552 | 20001127 <-- |
| US 6558885 | B1 | 20030506 | US 2000-721660 | 20001127 <-- |
| US 2004023170 | A1 | 20040205 | US 2003-385504 | 20030312 <-- |
| US 6852478 | B2 | 20050208 | | |

PRIORITY APPLN. INFO.: JP 1999-334982 A 19991125 <--
 JP 2000-92148 A 20000329 <--
 US 2000-721660 A3 20001127 <--

OTHER SOURCE(S): MARPAT 135:26820
 ED Entered STN: 08 Jun 2001
 GI



AB The photog. material has ≥ 1 magenta emulsion layer containing ≥ 1 pyrazotriazole-type coupler as a magenta dye former represented by I (Za, Zb = :CR4-, :N-; R1-4 = H, substituents; X = H, groups which is released by coupling reaction with oxidized developer), and the Ag halide emulsion of the magenta emulsion layer comprises ≥ 98 mol% AgCl. The photog. material has ≥ 1 nonphotosensitive hydrophilic colloidal layer containing dispersed solid dye microparticles represented by D-Xy (d = compound residue having coloring group; X = releasable H, group having releasable H; y = 1-7), and the magenta emulsion layer is placed farthest from the colloidal layer. The photog. material has high color reproducibility and is stably developed.

IT 172839-14-4

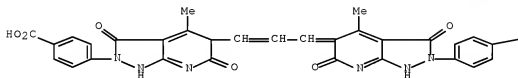
RL: DEV (Device component use); USES (Uses)

(silver halide photog. material containing pyrazotriazole-type magenta coupler and solid dye microparticle for high color reproducibility for movie)

RN 172839-14-4 HCAPLUS

CN Benzoic acid, 4-[5-[3-[2-(4-carboxyphenyl)-1,2,3,6-tetrahydro-4-methyl-3,6-dioxo-5H-pyrazolo[3,4-b]pyridin-5-ylidene]-1-propenyl]-1,3,5,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

—CO₂H

L41 ANSWER 11 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:841986 HCAPLUS Full-text

DOCUMENT NUMBER: 134:17506

TITLE: Preparation of pyrrolotriazines as kinases inhibitors for treating inflammation, cancer, and proliferative diseases

INVENTOR(S): Hunt, John T.; Bhide, Rajeev S.; Borzilleri, Robert M.; Qian, Ligang

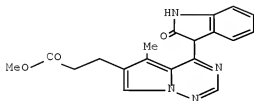
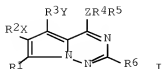
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

Serial No.:10/579,355

SOURCE: PCT Int. Appl., 130 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

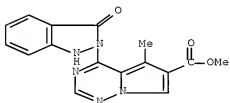
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|-----------------|
| WO 2000071129 | A1 | 20001130 | WO 2000-US13420 | 20000516 <-- |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2373990 | A1 | 20001130 | CA 2000-2373990 | 20000516 <-- |
| CA 2373990 | C | 20070508 | | |
| EP 1183033 | A1 | 20020306 | EP 2000-930761 | 20000516 <-- |
| EP 1183033 | B1 | 20060301 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY | | | | |
| BR 2000010482 | A | 20020423 | BR 2000-10482 | 20000516 <-- |
| JP 2003500359 | T | 20030107 | JP 2000-619433 | 20000516 <-- |
| HU 2003001005 | A2 | 20030728 | HU 2003-1005 | 20000516 <-- |
| HU 2003001005 | A3 | 20060529 | | |
| NZ 516292 | A | 20040130 | NZ 2000-516292 | 20000516 <-- |
| AU 770377 | B2 | 20040219 | AU 2000-48524 | 20000516 <-- |
| TR 200103352 | T2 | 20050321 | TR 2001-3352 | 20000516 <-- |
| AT 318603 | T | 20060315 | AT 2000-930761 | 20000516 <-- |
| EP 1669071 | A1 | 20060614 | EP 2006-3602 | 20000516 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| ES 2258459 | T3 | 20060901 | ES 2000-930761 | 20000516 <-- |
| TW 238163 | B | 20050821 | TW 2000-89109521 | 20000518 <-- |
| US 6982265 | B1 | 20060103 | US 2000-573829 | 20000518 <-- |
| IN 2001MN01414 | A | 20050304 | IN 2001-MN1414 | 20011113 <-- |
| MX 2001PA11832 | A | 20020621 | MX 2001-PA11832 | 20011119 <-- |
| NO 2001005650 | A | 20011120 | NO 2001-5650 | 20011120 <-- |
| NO 322214 | B1 | 20060828 | | |
| ZA 2001009577 | A | 20030220 | ZA 2001-9577 | 20011120 <-- |
| HK 1041599 | A1 | 20060915 | HK 2002-103297 | 20020502 <-- |
| US 2006004007 | A1 | 20060105 | US 2005-190412 | 20050727 <-- |
| US 7112675 | B2 | 20060926 | | |
| US 2006128709 | A1 | 20060615 | US 2006-345845 | 20060202 <-- |
| US 7244733 | B2 | 20070717 | | |
| PRIORITY APPLN. INFO.: | | | | |
| | | | US 1999-135265P | P 19990521 <-- |
| | | | US 2000-193727P | P 20000331 <-- |
| | | | EP 2000-930761 | A3 20000516 <-- |
| | | | WO 2000-US13420 | W 20000516 <-- |
| | | | US 2000-573829 | A3 20000518 <-- |
| | | | US 2005-190412 | A3 20050727 |

OTHER SOURCE(S): MARPAT 134:17506
 ED Entered STN: 01 Dec 2000
 GI



II

- AB Title compds. [I; X, Y independently = O, OCO, S, SO, SO₂, CO, CO₂, NH, NHCO, NHCONH, bond; Z = O, S, N, CH; R¹ = H, CH₃, OH, OCH₃, SH, SCH₃, NH₂, CO₂H, NO₂, CN, halo; R², R³ independently = H, alkyl, alkenyl, alkynyl, aryl, heterocyclo; R⁴, R⁵ independently = H, alkyl, aryl, heterocyclo; R⁴-R⁵ = monocyclic 5-7 membered cyclic ring, bicyclic 7-11 membered cyclic ring; R⁶ = H, alkyl, aryl, heterocyclo, halo], enantiomers, diastereomers, and pharmaceutically acceptable salts, prodrugs, carriers, and solvates, which inhibit the tyrosine kinase activity of growth factor receptors such as VEGFR-2, FGFR-1, PDGFR, HER-1, HER-2 and produce antiangiogenic effect, are prepared
- Title compds. I are useful as anti-cancer agents, antiinflammatories and agents for the treatment of diseases associated with signal transduction pathways operating through growth factor receptors. Thus, the title compound II was prepared
- IT 316443-16-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of pyrazolotriazines as kinases inhibitors useful in treating inflammation, cancer, and proliferative diseases)
- RN 310443-16-4 HCAPLUS
- CN Pyrrolo[2,1-f][1,2,4]triazine-6-carboxylic acid, 4-(1,3-dihydro-3-oxo-2H-indazol-2-yl)-5-methyl-, methyl ester (CA INDEX NAME)

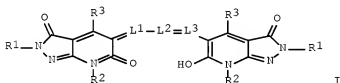


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 12 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:205746 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 132:258203

TITLE: Photothermographic material containing dye to be decolored on heating
 INVENTOR(S): Kamosaki, Toru
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 32 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| JP 2000089414 | A | 20000331 | JP 1998-252946 | 19980907 <-- |
| PRIORITY APPLN. INFO.: OTHER SOURCE(S): MARPAT 132:258203 | | | JP 1998-252946 | 19980907 <-- |
| ED Entered STN: 31 Mar 2000 | | | | |
| GI | | | | |



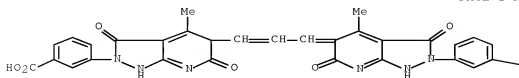
AB The material comprises photog. layers containing photosensitive Ag halide grains, a color developer (or its precursor), a coupler, and a binder and ≥ 1 Ag-containing light insensitive layer contains a conjugated methine dye I ($R_1 = H$, alkyl, aryl, heterocycle; $R_2 = H$, alkyl, aryl, heterocycle, COR4, SO2R4; $R_3 = H$, cyano, OH, COOH, alkyl, aryl, CO2R4, OR4, NR5R6, CONR5R6, NR5COR4, NR5SO2R4, NR5CONR5R6; $R_4 =$ alkyl, aryl; $R_5, R_6 = H$, alkyl, aryl; $L_1, L_2, L_3 =$ methine), which is decolored by reacting with a discoloring agent on heating. The material having the decoloring dye in antihalation layer, etc., shows improved color separation and sharpness after storage.

IT 262360-67-8 262360-69-8
 RL: TEM (Technical or engineered material use); USES (Uses)
 (photothermog. material involving nonphotosensitive layer containing conjugated methine dye to be decolored on heating)

RN 262360-67-8 HCAPLUS

CN Benzoic acid, 3-[5-[3-[2-(3-carboxyphenyl)-1,2,3,6-tetrahydro-4-methyl-3,6-dioxo-5H-pyrazolo[3,4-b]pyridin-5-ylidene]-1-propenyl]-1,3,5,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)

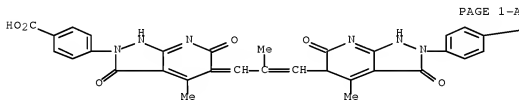
PAGE 1-A



PAGE 1-B

—CO₂H

RN 262360-69-0 HCAPLUS
 CN Benzoic acid, 4-[5-[3-[2-(4-carboxyphenyl)-1,2,3,6-tetrahydro-4-methyl-3,6-dioxo-5H-pyrazolo[3,4-b]pyridin-5-ylidene]-2-methyl-1-propenyl]-1,3,5,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)

—CO₂H

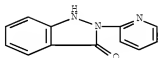
PAGE 1-B

L41 ANSWER 13 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1999:768118 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 132:92965
 TITLE: Electron ionization mass spectrometric studies of 1,2-dihydro-2-[2'-pyridyl, 4'-pyridyl and 2',6'-pyrimidyl]-3H-indazol-3-ones
 AUTHOR(S): Raza, Abdul R.; Rama, Nasim H.; Rehman, I.
 CORPORATE SOURCE: Department of Chemistry, Quaid-i-Azam University, Islamabad, 45320, Pak.
 SOURCE: Journal of the Chemical Society of Pakistan (1999), 21(1), 65-68
 CODEN: JCSPDF; ISSN: 0253-5106
 PUBLISHER: Chemical Society of Pakistan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 06 Dec 1999
 AB Electron-ionization mass spectra (EIMS) of 1,2-dihydro-2-(2-pyridyl-, 4-pyridyl and -2,6-pyrimidyl)-3H-indazol-3-ones and their related 2-nitrobenzamides are described. The mol. formulas are further confirmed by high-resolution EIMS matching of mol.-ion peaks.
 IT 74152-92-4, 3H-Indazol-3-one, 1,2-dihydro-2-(2-pyridinyl)-

255044-14-5, 1,2-Dihydro-2-(4-pyridinyl)-3H-indazol-3-one
 255044-15-6, 1,2-Dihydro-2-(2-pyrimidinyl)-3H-indazol-3-one
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC
 (Process); RACT (Reactant or reagent)
 (electron-ionization mass spectrometric studies of dihydropyridyl- and
 -pyrimidylindazolones and related nitrobenzamides)

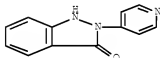
RN 74152-92-4 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(2-pyridinyl)- (CA INDEX NAME)



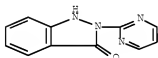
RN 255044-14-5 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-pyridinyl)- (CA INDEX NAME)



RN 255044-15-6 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(2-pyrimidinyl)- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 14 OF 132 HCAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1999:768115 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 132:92964

TITLE: Electron ionization mass spectrometric studies of
 1,2-dihydro-2-[2-(1,3-benzothiazolyl)]-3H-indazol-3-
 one and 1,2-dihydro-2-(3,4-dimethylphenyl)-6,7-
 dimethoxy-3H-indazol-3-one

AUTHOR(S): Raza, Abdul R.; Rama, Nasim H.; Rehman, I.

CORPORATE SOURCE: Department of Chemistry, Quaid-i-Azam University,
 Islamabad, 45320, Pak.

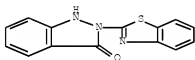
SOURCE: Journal of the Chemical Society of Pakistan (

1999), 21(1), 52-56

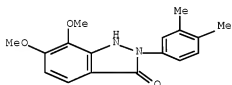
PUBLISHER: CODEN: JCSPDF; ISSN: 0253-5106

Chemical Society of Pakistan

DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 06 Dec 1999
 AB Electron-ionization mass spectra of the title compds. and their related compds. 2,3,4-N3R2C6H2CONHR1 (R = H, MeO; R1 = 1,3-benzothiazol-2-yl, 3,4-xylyl) are described using low-resolution electron-impact mass spectrometry (EIMS). The mol. formulas are further confirmed by high-resolution peak matching of mol.-ion peaks exhibited by EIMS.
 IT 175653-66-4, 3H-Indazol-3-one, 2-(2-benzothiazolyl)-1,2-dihydro-255044-20-3, 2-(3,4-Dimethylphenyl)-1,2-dihydro-6,7-dimethoxy-3H-indazol-3-one
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (electron-ionization mass spectra of dihydro(benzothiazolyl)- and -dimethoxy(dimethylphenyl)indazolones and related azidobenzamides)
 RN 175653-66-4 HCAPLUS
 CN 3H-Indazol-3-one, 2-(2-benzothiazolyl)-1,2-dihydro- (CA INDEX NAME)



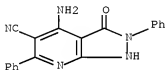
RN 255044-20-3 HCAPLUS
 CN 3H-Indazol-3-one, 2-(3,4-dimethylphenyl)-1,2-dihydro-6,7-dimethoxy- (CA INDEX NAME)



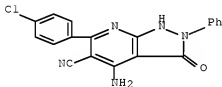
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 15 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1999;753648 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 132:151725
 TITLE: New synthesis of pyrazolo[3,4-b]pyridines
 AUTHOR(S): Youssef, A. M. S.
 CORPORATE SOURCE: Chemistry Department, Faculty of Science, University of Cairo, Giza, Egypt
 SOURCE: Egyptian Journal of Chemistry (1999), 42(3), 293-300
 CODEN: EGJCA3; ISSN: 0449-2285
 PUBLISHER: National Information and Documentation Centre
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 132:151725

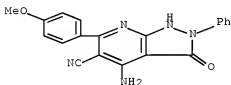
ED Entered STN: 28 Nov 1999
 AB Reaction of 3-amino-4,5-dihydro-1-phenyl-5-pyrazolone with ArCH:CRCN [Ar = Ph, 4-ClC₆H₄, 4-MeOC₆H₄, R = CN, CSNH₂, CO₂Et, Bz] gave pyrazolo[3,4-b]pyridinecarbonitriles.
 IT 257872-98-3P 257872-99-4P 257873-00-0P
 257873-01-1P 257873-02-2P 257873-03-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of pyrazolo[3,4-b]pyridinecarbonitriles)
 RN 257872-98-3 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 4-amino-2,3-dihydro-3-oxo-2,6-diphenyl- (CA INDEX NAME)



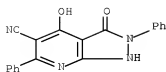
RN 257872-99-4 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 4-amino-6-(4-chlorophenyl)-2,3-dihydro-3-oxo-2-phenyl- (CA INDEX NAME)



RN 257873-00-0 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 4-amino-2,3-dihydro-6-(4-methoxyphenyl)-3-oxo-2-phenyl- (CA INDEX NAME)

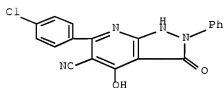


RN 257873-01-1 HCAPLUS
 CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 2,3-dihydro-4-hydroxy-3-oxo-2,6-diphenyl- (CA INDEX NAME)



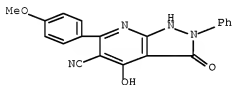
RN 257873-02-2 HCAPLUS

CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 6-(4-chlorophenyl)-2,3-dihydro-4-hydroxy-3-oxo-2-phenyl- (CA INDEX NAME)



RN 257873-03-3 HCAPLUS

CN 1H-Pyrazolo[3,4-b]pyridine-5-carbonitrile, 2,3-dihydro-4-hydroxy-6-(4-methoxyphenyl)-3-oxo-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 60 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1989:214752 HCAPLUS Full-text
 DOCUMENT NUMBER: 110:214752
 TITLE: Polyazo and disazo reactive dyes and their use
 INVENTOR(S): Herd, Karl Josef
 PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
 SOURCE: Eur. Pat. Appl., 28 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO.

DATE

| | | | | |
|-----------|----|----------|----------------|--------------|
| EP 292825 | A2 | 19881130 | EP 1988-107805 | 19880516 <-- |
| EP 292825 | A3 | 19890308 | | |
| EP 292825 | B1 | 19910807 | | |

R: CH, DE, FR, GB, LI

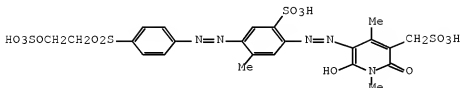
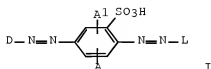
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|-------------|----|----------|-----------------|--------------|
| DE 3717814 | A1 | 19881208 | DE 1987-3717814 | 19870527 <-- |
| US 5093484 | A | 19920303 | US 1988-196168 | 19880518 <-- |
| JP 63309560 | A | 19881216 | JP 1988-124040 | 19880523 <-- |

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 110:214752

ED Entered STN: 10 Jun 1989

GI



II

AB Disazo reactive dyes I [A, A1 = H, C1-4 alkyl, C1-4 alkoxy, halogen; D = fiber-reactive group-containing (un)substituted Ph or naphthyl residue; L = coupling component residue], useful for dyeing or printing hydroxyl and/or carbonamide group-containing fabrics, are prepared 4'-(β-Hydroxyethylsulfonyl)-2-methyl-4-aminoazobenzene was sulfonated with oleum and the intermediate diazotized and coupled with 3-(aminocarbonyl)-1,4-dimethyl-5-sulfomethyl-6-hydroxy-2-pyridone Na salt, forming II, λ_{max} 455 nm, which dyed wool in a fast orange-yellow shade.

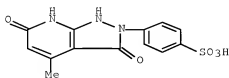
IT 86104-85-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling of, with diazotized (sulfatoethylsulfonyl)methylsulfoaminoazo benzene)

RN 86104-85-0 HCAPLUS

CN Benzenesulfonic acid, 4-(1,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl)- (CA INDEX NAME)

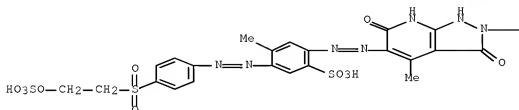


IT 119894-82-6P

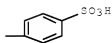
RL: PREP (Preparation)
(manufacture of, as reactive brown dye)

RN 119894-83-6 HCAPLUS
CN Benzenesulfonic acid, 4-methyl-5-[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]-2-[[2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-(4-sulphophenyl)-1H-pyrazolo[3,4-b]pyridin-5-yl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



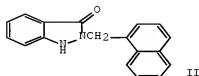
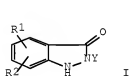
L41 ANSWER 61 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:192811 HCAPLUS Full-text
DOCUMENT NUMBER: 110:192811
TITLE: Preparation of 1,2-dihydro-3H-indazol-3-ones as lipoxigenase inhibitors.
INVENTOR(S): Bruneau, Pierre Andre Raymond; Carey, Frank; Delvare, Christian Robert Ernest; Gibson, Keith Hopkinson; McMillan, Rodger Martin
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK; ICI Pharma S. A.
SOURCE: Eur. Pat. Appl., 90 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| EP 284174 | A1 | 19880928 | EP 1988-300281 | 19880114 <-- |
| EP 284174 | B1 | 19920729 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| IL 84944 | A | 19920216 | IL 1987-84944 | 19871225 <-- |
| AU 8783175 | A | 19880721 | AU 1987-83175 | 19871231 <-- |
| AU 606112 | B2 | 19910131 | | |
| ZA 8800046 | A | 19880831 | ZA 1988-46 | 19880105 <-- |
| FI 8800195 | A | 19880720 | FI 1988-195 | 19880118 <-- |
| NO 8800182 | A | 19880720 | NO 1988-182 | 19880118 <-- |
| JP 63253069 | A | 19881020 | JP 1988-7096 | 19880118 <-- |

Serial No.:10/579,355

| | | | | |
|------------------------|---|----------|----------------|-----------------|
| DK 8800228 | A | 19880720 | DK 1988-228 | 19880119 <-- |
| US 5173496 | A | 19921222 | US 1992-863333 | 19920402 <-- |
| PRIORITY APPLN. INFO.: | | | EP 1987-400122 | A 19870119 <-- |
| | | | EP 1987-401798 | A 19870731 <-- |
| | | | US 1988-143373 | B1 19880113 <-- |
| | | | US 1990-532348 | B1 19900605 <-- |

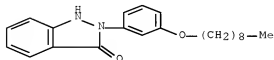
OTHER SOURCE(S): MARPAT 110:192811
 ED Entered STN: 26 May 1989
 GI



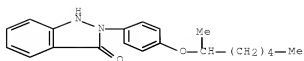
AB Dihydroindazolines I (R1 = H, halo, NO2, OH, C2-6 alkanoyloxy, C1-6 alkyl, C1-6 alkoxy, C1-4 fluoroalkyl, C2-6 alkanoyl, NH2, C1-6 alkylamino, di(C1-4 alkyl)amino, C2-6 alkanoylamino, C1-6 hydroxyalkyl; R2 = H, halo, C1-6 alkyl, C1-6 alkoxy; Y = wide variety of substituents), many of which are new, are useful as 5-lipoxygenase inhibitors. Reductive cyclization of N-(1-naphthylmethyl)-2-nitrobenzamide by powdered Zn and NaOH in ag. MeOH gave dihydro(naphthylmethyl)indazoline II. In an in vitro assay using heparinized rat blood and challenge by the Ca ionophore A23187, II had IC50 values of 0.8 μ M vs. LTB4 and 100 μ M vs. PGE2.

IT 120273-69-0P 120273-73-6P 120273-75-6P
 120273-83-8P 120273-86-1P 120273-87-2P
 120273-91-6P 120273-93-0P 120273-94-1P
 120274-01-3P 120274-04-6P 120274-06-8P
 120274-07-9P 120274-08-0P 120274-12-6P
 120274-13-7P 120274-14-8P 120274-16-0P
 120274-17-1P 120274-64-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as lipoxygenase inhibitor)

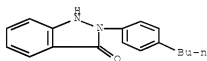
RN 120273-69-0 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-2-[3-(nonyloxy)phenyl]- (CA INDEX NAME)



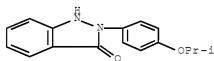
RN 120273-73-6 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-2-[4-[(1-methylhexyl)oxy]phenyl]- (CA INDEX NAME)



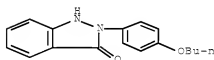
RN 120273-75-8 HCAPLUS
 CN 3H-Indazol-3-one, 2-(4-butylphenyl)-1,2-dihydro- (CA INDEX NAME)



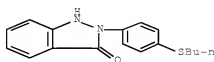
RN 120273-83-8 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-2-[4-(1-methylethoxy)phenyl]- (CA INDEX NAME)



RN 120273-86-1 HCAPLUS
 CN 3H-Indazol-3-one, 2-(4-butoxyphenyl)-1,2-dihydro- (CA INDEX NAME)

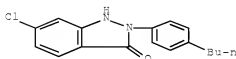


RN 120273-87-2 HCAPLUS
 CN 3H-Indazol-3-one, 2-[4-(butylthio)phenyl]-1,2-dihydro- (CA INDEX NAME)



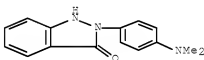
RN 120273-91-8 HCAPLUS

CN 3H-Indazol-3-one, 2-(4-butylphenyl)-6-chloro-1,2-dihydro- (CA INDEX NAME)



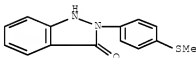
RN 120273-93-0 HCAPLUS

CN 3H-Indazol-3-one, 2-[4-(dimethylamino)phenyl]-1,2-dihydro- (CA INDEX NAME)



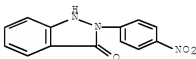
RN 120273-94-1 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-[4-(methylthio)phenyl]- (CA INDEX NAME)



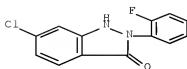
RN 120274-01-3 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-nitrophenyl)- (CA INDEX NAME)



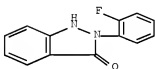
RN 120274-04-6 HCAPLUS

CN 3H-Indazol-3-one, 6-chloro-2-(2-fluorophenyl)-1,2-dihydro- (CA INDEX NAME)



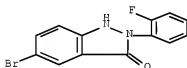
RN 120274-06-8 HCAPLUS

CN 3H-Indazol-3-one, 2-(2-fluorophenyl)-1,2-dihydro- (CA INDEX NAME)



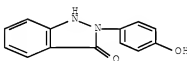
RN 120274-07-9 HCAPLUS

CN 3H-Indazol-3-one, 5-bromo-2-(2-fluorophenyl)-1,2-dihydro- (CA INDEX NAME)



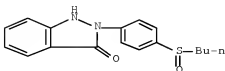
RN 120274-08-0 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-hydroxyphenyl)- (CA INDEX NAME)



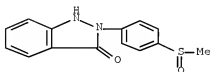
RN 120274-12-6 HCAPLUS

CN 3H-Indazol-3-one, 2-[4-(butylsulfinyl)phenyl]-1,2-dihydro- (CA INDEX NAME)



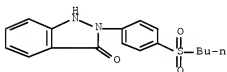
RN 120274-13-7 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-[4-(methylsulfonyl)phenyl]- (CA INDEX NAME)



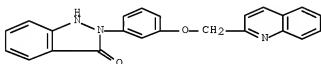
RN 120274-14-8 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-[4-(butylsulfonyl)phenyl]-1,2-dihydro- (CA INDEX NAME)



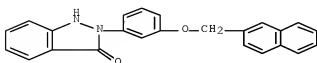
RN 120274-16-0 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-[3-(2-quinolinylmethoxy)phenyl]- (CA INDEX NAME)



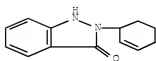
RN 120274-17-1 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-[3-(2-naphthalenylmethoxy)phenyl]- (CA INDEX NAME)



RN 120274-64-8 HCAPLUS

CN 3H-Indazol-3-one, 2-(2-cyclohexen-1-yl)-1,2-dihydro- (CA INDEX NAME)

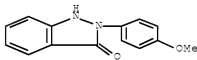


IT 74152-89-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in synthesis of lipoxxygenase-inhibiting
 dihydroindazolones)

RN 74152-89-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-methoxyphenyl)- (CA INDEX NAME)



L41 ANSWER 62 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:492072 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 109:92072

TITLE: Thermal rearrangement of 2-aryl-1-cyanoindazol-3-ones

AUTHOR(S): Bird, C. W.; Kapili, M.

CORPORATE SOURCE: Dep. Chem., King's Coll., London, W8 7AH, UK

SOURCE: Tetrahedron (1987), 43(20), 4621-4

CODEN: TETRA; ISSN: 0040-4020

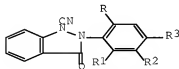
DOCUMENT TYPE: Journal

LANGUAGE: English

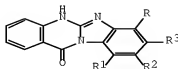
OTHER SOURCE(S): CASREACT 109:92072

ED Entered STN: 17 Sep 1988

GI



I



II

AB 2-Aryl-1-cyanoindazol-3-ones (I; R, R1, R2 = H, Me; R3 = H, Cl, Me, OMe) were prepared, and their thermal rearrangement to the corresponding

benzimidazo[2,1-b]quinazolones (II) was examined Quant. studies using differential scanning calorimetry provided rates, energies and entropies of activation. The rates of rearrangement of the 2-(p-substituted phenyl) compds. are correlated to the Hammett relationship by using σ^+ substituent consts. In the case of the 2-(2,6-dimethylphenyl) and 2-(2,4,6-trimethylphenyl) compds. rearrangement is accompanied by [1,9] sigmatropic shifts of the obstructing Me groups.

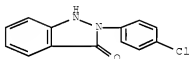
IT 17049-63-7 74152-87-7 74152-88-8

74152-89-9 74152-91-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation)

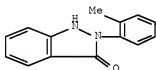
RN 17049-63-7 HCAPLUS

CN 3H-Indazol-3-one, 2-(4-chlorophenyl)-1,2-dihydro- (CA INDEX NAME)



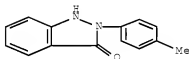
RN 74152-87-7 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(2-methylphenyl)- (CA INDEX NAME)



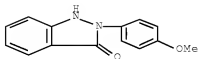
RN 74152-88-8 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-methylphenyl)- (CA INDEX NAME)



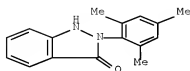
RN 74152-89-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-methoxyphenyl)- (CA INDEX NAME)



RN 74152-91-3 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(2,4,6-trimethylphenyl)- (CA INDEX NAME)

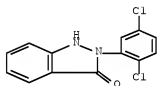


IT 115819-39-1P 115819-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and attempted cyanation of)

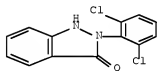
RN 115819-39-1 HCAPLUS

CN 3H-Indazol-3-one, 2-(2,5-dichlorophenyl)-1,2-dihydro- (CA INDEX NAME)



RN 115819-40-4 HCAPLUS

CN 3H-Indazol-3-one, 2-(2,6-dichlorophenyl)-1,2-dihydro- (CA INDEX NAME)

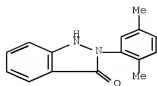


IT 115819-37-9P 115819-38-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyanation of)

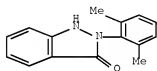
RN 115819-37-9 HCAPLUS

CN 3H-Indazol-3-one, 2-(2,5-dimethylphenyl)-1,2-dihydro- (CA INDEX NAME)



RN 115819-38-0 HCAPLUS

CN 3H-Indazol-3-one, 2-(2,6-dimethylphenyl)-1,2-dihydro- (CA INDEX NAME)

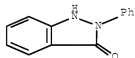


IT 17049-65-9P

RL: SPN (Synthetic preparation); PREP (Preparation of)
(preparation of)

RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 63 OF 132 HCAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1988:37827 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 108:37827

TITLE: Preparation of chlorofluorobenzothiazolonyltetrahydroindazoles as herbicides

INVENTOR(S): Haga, Toru; Nagano, Eiki; Morita, Kouichi; Sato, Ryo

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 20 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|--------------|
| ----- | | ----- | ----- | ----- |
| EP 235567 | A2 | 19870909 | EP 1987-101138 | 19870128 <-- |
| EP 235567 | A3 | 19910109 | | |
| EP 235567 | B1 | 19940112 | | |

R: DE, GB, IT

Serial No.:10/579,355

| | | | | |
|-------------|----|----------|----------------|--------------|
| JP 62238268 | A | 19871019 | JP 1986-79661 | 19860407 <-- |
| JP 62238284 | A | 19871019 | JP 1986-79662 | 19860407 <-- |
| JP 06067931 | B | 19940831 | | |
| JP 62238285 | A | 19871019 | JP 1986-79663 | 19860407 <-- |
| JP 06067932 | B | 19940831 | | |
| JP 62238269 | A | 19871019 | JP 1986-81420 | 19860409 <-- |
| JP 62238270 | A | 19871019 | JP 1986-81421 | 19860409 <-- |
| JP 62252787 | A | 19871104 | JP 1987-12846 | 19870122 <-- |
| JP 07100703 | B | 19951101 | | |
| US 4820333 | A | 19890411 | US 1987-8314 | 19870129 <-- |
| US 4831150 | A | 19890516 | US 1988-203906 | 19880608 <-- |
| US 4831149 | A | 19890516 | US 1988-204018 | 19880608 <-- |
| JP 06321922 | A | 19941122 | JP 1994-248 | 19940106 <-- |
| JP 2503930 | B2 | 19960605 | | |

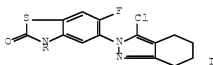
PRIORITY APPLN. INFO.:

| | | | | |
|--|--|---------------|----|--------------|
| | | JP 1986-19044 | A | 19860129 <-- |
| | | JP 1986-79661 | A | 19860407 <-- |
| | | JP 1986-79662 | A | 19860407 <-- |
| | | JP 1986-79663 | A | 19860407 <-- |
| | | JP 1986-81420 | A | 19860409 <-- |
| | | JP 1986-81421 | A | 19860409 <-- |
| | | JP 1987-12846 | | 19870122 <-- |
| | | US 1987-8314 | A3 | 19870129 <-- |

OTHER SOURCE(S): CASREACT 108:37827

ED Entered SIN: 06 Feb 1988

GI

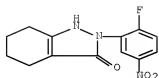


AB The title compds. [I; R = C1-5 alkyl, C3-4 alkenyl, C3-4 alkynyl, C1-3 alkoxy (C1-2)alkyl] were prepared as herbicides. I (R = H) was added to a suspension of NaH in DMF at 0° and the mixture was stirred 30 min. BrCH₂C.tplbond.CH was added and the mixture was heated at 50-60° for 2-3 h to give I (R = CH₂C.tplbond.CH) (II). At 40 g/are preemergent I gave complete control of velvetleaf. A wettable powder was prepared containing 50 parts II, 3 parts Ca ligninsulfonate, 2 parts Na laurylsulfate, and 45 parts hydrated silica by weight

IT 112269-53-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and chlorination of, by trichloromethyl chloroformate)

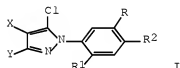
RN 112269-53-1 HCAPLUS

CN 3H-Indazol-3-one, 2-(2-fluoro-5-nitrophenyl)-1,2,4,5,6,7-hexahydro- (CA INDEX NAME)



L41 ANSWER 64 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:576060 HCAPLUS Full-text
 DOCUMENT NUMBER: 107:176060
 TITLE: Preparation of 1-(3-aminophenyl)pyrazoles as
 herbicides and herbicide intermediates
 INVENTOR(S): Kawada, Shuji; Kobayashi, Shinichi; Yanagi, Mikio
 PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------|------|----------|---------------------|--------------|
| JP 62123173 | A | 19870604 | JP 1985-262576 | 19851125 <-- |
| PRIORITY APPLN. INFO.: | | | JP 1985-262576 | 19851125 <-- |
| OTHER SOURCE(S): | | | CASREACT 107:176060 | |
| ED Entered STN: 14 Nov 1987 | | | | |
| GI | | | | |

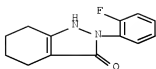


AB The title compds. [I; R = NH₂; R₁, R₂, X, Y = H, halo, alkyl; XY = (CH₂)_n; n = 3, 4], useful as herbicides and herbicide intermediates (no data), were prep'd by nitration of I (R = H) and reduction of the resulting I (R = NO₂). HNO₃ and concentrated H₂SO₄ were added dropwise at -5° to a solution of I (R = H, R₁ = F, R₂ = Cl, X = Br, Y = Me) and the mixture stirred 4 h at -5° to give 88% I (R = NO₂, R₁ = F, R₂ = Cl, X = Br, Y = Me) which was reduced by Fe/HCl to give 86% I (R = NH₂, R₁ = F, R₂ = Cl, X = Br, Y = Me).

IT 110706-34-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and chlorination of)

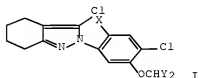
RN 110706-34-8 HCAPLUS

CN 3H-Indazol-3-one, 2-(2-fluorophenyl)-1,2,4,5,6,7-hexahydro- (CA INDEX NAME)



L41 ANSWER 65 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:98110 HCAPLUS Full-text
 DOCUMENT NUMBER: 106:98110
 TITLE: Preparation of 4,5,6,7-tetrahydro-2H-indazole derivatives and herbicides containing them
 INVENTOR(S): Hayase, Yoshio; Ohtsuka, Toshikazu; Ide, Kinya; Takahashi, Toshio
 PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 24 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------|------|--------------------------------------|-----------------|--------------|
| EP 197495 | A1 | 19861015 | EP 1986-104455 | 19860402 <-- |
| EP 197495 | B1 | 19900711 | | |
| R: DE, FR, IT | | | | |
| US 4695312 | A | 19870922 | US 1986-846051 | 19860331 <-- |
| JP 62030761 | A | 19870209 | JP 1986-77452 | 19860402 <-- |
| JP 05075747 | B | 19931021 | | |
| GB 2173501 | A | 19861015 | GB 1986-8198 | 19860403 <-- |
| GB 2173501 | B | 19880817 | | |
| PRIORITY APPLN. INFO.: | | JP 1985-71428 | A | 19850403 <-- |
| OTHER SOURCE(S): | | CASREACT 106:98110; MARPAT 106:98110 | | |
| ED Entered SIN: 05 Apr 1987 | | | | |
| GI | | | | |

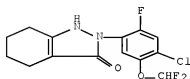


AB The title compds. I (X, Y = halo) are prepared as herbicides. Thus, 3-chloro-2-(2,4-dichloro-5-hydroxyphenyl)-4,5,6,7-tetrahydro-2H-indazole was reacted with ClCH₂F₂, in NaOH-containing dioxane, at 50-60°, to give I (X = Cl, Y = F) (II). Pre-emergence 10 g II/are totally controlled large crabgrass and slender amaranth, with no injury to wheat, soybean, and cotton.

IT 106969-05-5P 106969-08-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

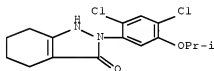
(preparation and chlorination of)

RN 106969-05-5 HCAPLUS

CN 3H-Indazol-3-one, 2-[4-chloro-5-(difluoromethoxy)-2-fluorophenyl]-
1,2,4,5,6,7-hexahydro- (CA INDEX NAME)

RN 106969-08-8 HCAPLUS

CN 3H-Indazol-3-one, 2-[2,4-dichloro-5-(1-methylethoxy)phenyl]-1,2,4,5,6,7-hexahydro- (CA INDEX NAME)



L41 ANSWER 66 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:626551 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 105:226551

ORIGINAL REFERENCE NO.: 105:36587a,36590a

TITLE: (Sulfonamidophenyl)pyrazoles and their use as herbicides

INVENTOR(S): Yanagi, Mikio; Kawada, Shuji; Futatsuya, Fumio; Kobayashi, Kenji

PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 39 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

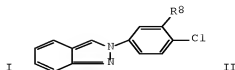
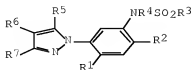
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------|------|----------|-----------------|----------------|
| EP 191303 | A1 | 19860820 | EP 1986-100385 | 19860114 <-- |
| R: CH, DE, FR, GB, IT, LI | | | | |
| JP 61165374 | A | 19860726 | JP 1985-3957 | 19850116 <-- |
| JP 62033155 | A | 19870213 | JP 1985-171793 | 19850806 <-- |
| US 4666507 | A | 19870519 | US 1985-814395 | 19851230 <-- |
| BR 8600123 | A | 19860923 | BR 1986-123 | 19860115 <-- |
| NL 8601766 | A | 19870302 | NL 1986-1766 | 19860707 <-- |
| BE 905091 | A1 | 19870112 | BE 1986-216907 | 19860711 <-- |
| ES 2000669 | A6 | 19880316 | ES 1986-302 | 19860715 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| | | | JP 1985-3957 | A 19850116 <-- |
| | | | JP 1985-171793 | A 19850806 <-- |

OTHER SOURCE(S): CASREACT 105:226551; MARPAT 105:226551
 ED Entered STN: 26 Dec 1986
 GI



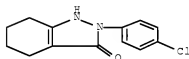
AB The title compds. [I; R1 = H, halo, Me; R2 = H, halo, alkyl; R3 = PhCH2, (substituted) lower alkyl, Ph; R4 = H, alkenyl, alkynyl, (substituted) alkyl, (halo-substituted) MeSO2, Ph; R5 = halo; R6, R7 = Me, Et; R6R7 = (CH2)3, (CH2)4] (.apprx.64 compds.) were prepared as herbicides. Thus, benzopyrazole II (R8 = NO2) was reduced to the amine which was treated with (F3CSO2)2O to give 50% II (R8 = NHSO2CF3) (III). At 0.8 g/are, III gave complete control of barnyardgrass, broadleaf weeds, and bulrush, without damage to preemegent rice in flooded fields. The title compds. also controlled weeds in soybeans, cotton, corn, wheat, and sunflowers without damage to crops.

IT 54486-21-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of)

RN 64486-21-1 HCAPLUS

CN 3H-Indazol-3-one, 2-(4-chlorophenyl)-1,2,4,5,6,7-hexahydro- (CA INDEX NAME)



L41 ANSWER 67 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:148872 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 104:148872

ORIGINAL REFERENCE NO.: 104:23569a,23572a

TITLE: Tetrahydroindazoles

INVENTOR(S): Naohara, Tetsuo; Natsume, Fumitsugu; Yotsuya,

Toyohiko; Suzuki, Seichi; Kabe, Hiroshi

PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

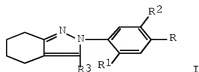
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

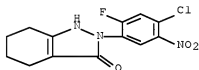
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|-------|-----------------|-------|
| ----- | ---- | ----- | ----- | ----- |

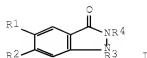
JP 60233061 A 19851119 JP 1984-89665 19840504 <--
 PRIORITY APPLN. INFO.: JP 1984-89665 19840504 <--
 OTHER SOURCE(S): CASREACT 104:148872
 ED Entered STN: 03 May 1986
 GI



AB The title compds. [I, R = Cl, Br; R1 = F, Cl, MeO; R2 = NO2, substituted amino or sulfonyl, sulfinyl, or sulfinyl; R3 = halo, MeO], useful as herbicides (effective at 5,10,20 g/are), were prepared. Thus, refluxing a mixture of 15.0 g 2-(4-chloro-2-fluoro-5-nitrophenyl)-1,2,4,5,6,7-hexahydro-3H-indazol-3-one and 11.6 g POCl3 for 5 h gave 5.80 g I [R = R3 = Cl, R1 = F, R2 = NO2].
 IT 101303-75-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of)
 RN 101303-75-7 HCAPLUS
 CN 3H-Indazol-3-one, 2-(4-chloro-2-fluoro-5-nitrophenyl)-1,2,4,5,6,7-hexahydro- (CA INDEX NAME)



L41 ANSWER 68 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1984:203128 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 100:203128
 ORIGINAL REFERENCE NO.: 100:30709a,30712a
 TITLE: Hypolipidemic activity of phthalimide derivatives. 7.
 Structure-activity studies of indazolone analogs
 AUTHOR(S): Wyrick, Steven D.; Voorstad, P. Josee; Cocolas, George; Hall, Iris H.
 CORPORATE SOURCE: Sch. Pharm., Univ. North Carolina, Chapel Hill, NC, 27514, USA
 SOURCE: Journal of Medicinal Chemistry (1984), 27(6), 768-72
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 23 Jun 1984
 GI

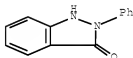


AB The indazolone analogs I (R1 = H, Cl, or Me; R2 = H or Cl; R3 = H or CO2Et; R4 = H, C1-5 alkyl, CO2Et, CH2CH2OH, CH2(CH2)2OH, CH2CH2C(O)Me, Ph, (un)substituted benzyl) prepared from the corresponding anthranilic acid by diazotization, alkylation, and decarboxylation, were evaluated for antihyperlipidemic activity in CF1 male mice at 20 mg/kg/day, i.p. N2-Butylindazolone (I; R1 = R2 = R3 = H, R4 = Bu) [89438-55-1] was the most active compound. Structure activity relations are discussed.

IT 17049-65-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and hypolipemic activity of)

RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 69 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:596653 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 99:196653

ORIGINAL REFERENCE NO.: 99:30279a,30282a

TITLE: Methine dyes

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF

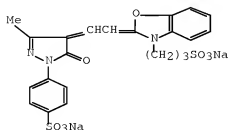
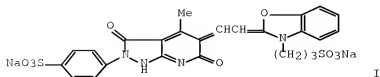
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------|------|----------|-----------------|--------------|
| JP 58065756 | A | 19830419 | JP 1981-162971 | 19811012 <-- |
| JP 59005622 | B | 19840206 | | |
| PRIORITY APPLN. INFO.: | | | JP 1981-162971 | 19811012 <-- |
| ED Entered STN: 12 May 1984 | | | | |
| GI | | | | |



AB Pyrazolopyridine ring-containing methines absorbing at longer wavelength than conventional pyrazolinone analogs were prepared. These methines form stable solns. and are irreversibly bleached in photog. processes. Thus, 4-methyl-2-(4-sulfophenyl)pyrazolo[3,4-b]pyridine-3,6-dione triethylamine salt [65563-44-2] was treated with anhydro-2-(2-anilino vinyl)-3- (3-sulfopropyl)benzoxazolium hydroxide [55036-57-2] in γ -butyrolactone, Ac₂O, and then Et₃N, refluxed for 15 min, filtered, and treated with methanolic NaI to give red-orange I [65563-31-7], λ_{max} (H₂O) 484 nm, compared with 446 nm for II.

IT 65563-44-2

RL: USES (Uses)
(in methine dye manufacture)

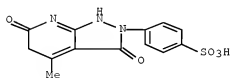
RN 65563-44-2 HCAPLUS

CN Benzenesulfonic acid, 4-(1,3,5,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 65563-43-1

CMF C13 H11 N3 O5 S



CM 2

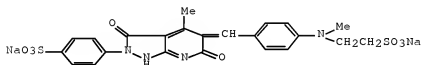
CRN 121-44-8

CMF C6 H15 N



L41 ANSWER 70 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1983:559944 HCAPLUS Full-text
 DOCUMENT NUMBER: 99:159944
 ORIGINAL REFERENCE NO.: 99:24523a,24526a
 TITLE: Methine dyes
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------|------|----------|-----------------|--------------|
| JP 58065757 | A | 19830419 | JP 1981-162972 | 19811012 <-- |
| PRIORITY APPLN. INFO.: | | | JP 1981-162972 | 19811012 <-- |
| ED Entered STN: 12 May 1984 | | | | |
| GI | | | | |



I

AB Pyrazolopyridine methine dyes showing absorption at long wavelength region were prepared. These dyes were irreversibly bleached by sulfite and used in photog. materials without inducing fogging or sensitivity lowering. Thus, 4-methyl-2-(4-sulfophenyl)pyrazolo[3,4-b]pyridine-3,6-dione triethylamine salt [65563-44-2] was treated with 4-[N-methyl-N-(2-sulfoethyl)amino]benzaldehyde Na salt [56405-41-5] in the presence of Et3N in γ -butyrolactone for 5 min, treated with AcOH at 150° for 15 min, and stirred with NaI for 10 min to give dark red I [65563-39-5], λ_{\max} (H2O) 600 nm.

IT 65563-44-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with [methyl(sulfoethyl)amino]benzaldehyde)

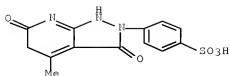
RN 65563-44-2 HCAPLUS

CN Benzenesulfonic acid, 4-(1,3,5,6-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl)-, compd. with N,N-diethylethanamine (1:1)
 (9CI) (CA INDEX NAME)

CM 1

CRN 65563-43-1

CMF C13 H11 N3 O5 S



CM 2

CRN 121-44-8

CMF C6 H15 N



L41 ANSWER 71 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:558316 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 99:158316

ORIGINAL REFERENCE NO.: 99:24273a,24276a

TITLE: Comparative study of the reactivity of ethyl acetoacetate and ethyl 3-aminocrotonate with pyrazolone derivatives

AUTHOR(S): Maquestiau, A.; Van Haverbeke, Y.; Vanden Eynde, J. J.

CORPORATE SOURCE: Lab. Chim. Org., Univ. Etat, Mons, 7000, Belg.

SOURCE: Bulletin des Societes Chimiques Belges (1983), 92(5), 451-8

CODEN: BSCBAG; ISSN: 0037-9646

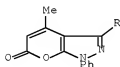
DOCUMENT TYPE: Journal

LANGUAGE: French

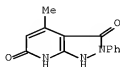
OTHER SOURCE(S): CASREACT 99:158316

ED Entered STN: 12 May 1984

GI



I



II

AB Pyrazolinone and pyrazolidinedione compds. reacted with $\text{MeCOCH}_2\text{CO}_2\text{Et}$ and $\text{MeC}(\text{NH}_2):\text{CHCO}_2\text{Et}$ to yield pyranopyrazoles I (R = Me, OH). 1-Phenyl-3-methyl-2-pyrazolin-5-one was treated with $\text{MeCOCH}_2\text{CO}_2\text{Et}$ (or its enamine) to give I (R =

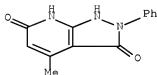
Me). Pyrazolopyridine derivative II was obtained from 1-phenyl-3-amino-2-pyrazolin-5-one and MeCOCH₂CO₂Et (or its enamine).

IT 71290-80-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71290-80-7 HCAPLUS

CN 1H-Pyrazolo[3,4-b]pyridine-3,6(2H,7H)-dione, 4-methyl-2-phenyl- (CA INDEX NAME)



L41 ANSWER 72 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:424020 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 99:24020

ORIGINAL REFERENCE NO.: 99:3887a,3890a

TITLE: 3,6-Dioxo-1,2-dihydro-7H-pyrazolo[3,4-b]pyridine azo dyes

INVENTOR(S): Herd, Karl Josef

PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.

SOURCE: Ger. Offen., '72 pp.

CODEN: GWXXBX

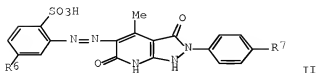
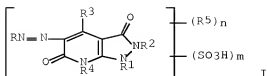
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| DE 3138774 | A1 | 19830414 | DE 1981-3138774 | 19810930 <-- |
| EP 75808 | A2 | 19830406 | EP 1982-108615 | 19820918 <-- |
| EP 75808 | A3 | 19830727 | | |
| R: CH, DE, FR, GB, IT, LI | | | | |
| JP 58069254 | A | 19830425 | JP 1982-166783 | 19820927 <-- |
| PRIORITY APPLN. INFO.: DE 1981-3138774 A 19810930 <-- | | | | |
| OTHER SOURCE(S): MARPAT 99:24020 | | | | |
| ED Entered STN: 12 May 1984 | | | | |
| GI | | | | |



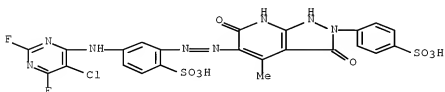
AB Dyes of general structure I are prepared, where R represents the residue of a benzene, naphthalene, or heterocyclic diazo component; R1 and R2 = H, acyl, optionally substituted alkyl, aryl, heteroaryl, or aralkyl, or O-, NH-, SO-, or SO2-interrupted alkenyl; R3 = H, optionally substituted alkyl or aryl, carboxylate ester, carbamoyl, amino, or optionally substituted heteroaryl; R4 = H, optionally substituted alkyl or aryl, alkenyl, OH, or acylamino; R5 = fiber-reactive group; n = 0-2; and m = 0-6. I in which m ≠ 0 are reactive dyes for cellulose and polyamide fiber, and those with n = 0 which are water soluble are dyes for wool, nylon, leather, and cellulosic fibers. Typical dyes are brown (on nylon and wool) II (R6 = R7 = H) [86104-89-4], prepared by coupling diazotized 2-H2NC6H4SO3H [88-21-1] with 4-methyl-2-phenyl-1,2-dihydro-7H-pyrazolo[3,4-b]pyridine-3,6-dione [71290-80-7], and yellowish brown (on cellulose) II (R6 = 5-chloro-2,6-difluoropyrimidin-4-ylamino, R7 = SO3H) [86104-90-7], prepared by coupling diazotized 2-amino-4-[(5-chloro-2,6-difluoropyrimidin-4-yl)amino]benzenesulfonic acid [26592-28-9] with 4-methyl-2-(4-sulfophenyl)-1,2-dihydro-7H-pyrazolo[3,4-b]pyridine-3,6-dione [86104-85-0].

IT 86104-90-7

RL: TEM (Technical or engineered material use); USES (Uses)
(dye, for cellulosic textiles, manufacture of)

RN 86104-90-7 HCAPLUS

CN Benzenesulfonic acid, 4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]-2-[[2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-(4-sulfophenyl)-1H-pyrazolo[3,4-b]pyridin-5-yl]azo]- (9CI) (CA INDEX NAME)

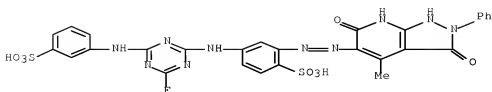


IT 86104-77-0 86104-78-1

RL: TEM (Technical or engineered material use); USES (Uses)
(dye, for cotton)

RN 86104-77-0 HCAPLUS

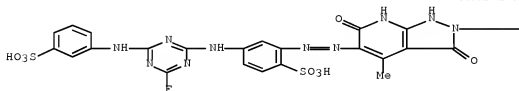
CN Benzenesulfonic acid, 4-[[4-fluoro-6-[(3-sulfophenyl)amino]-1,3,5-triazin-2-yl]amino]-2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



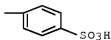
RN 86104-78-1 HCAPLUS

CN Benzenesulfonic acid, 5-[[[4-fluoro-6-[(3-sulfophenyl)amino]-1,3,5-triazin-2-yl]amino]-2-[[[2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-(4-sulfophenyl)-1H-pyrazolo[3,4-b]pyridin-5-yl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

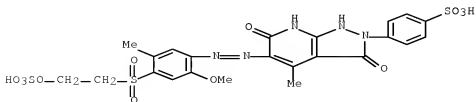


IT 86104-79-2

RL: TEM (Technical or engineered material use); USES (Uses)
(dye, for cotton, manufacture of)

RN 86104-79-2 HCAPLUS

CN Benzenesulfonic acid, 4-[[[1,3,6,7-tetrahydro-5-[[[2-methoxy-5-methyl-4-[[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)



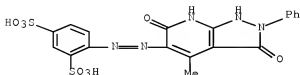
IT 86104-50-9

RL: USES (Uses)

(dye, for leather, manufacture of)

RN 86104-50-9 HCAPLUS

CN 1,3-Benzenedisulfonic acid, 4-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



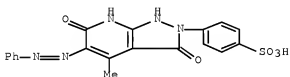
IT 86104-63-4 86104-89-4

RL: USES (Uses)

(dye, for nylon and wool, manufacture of)

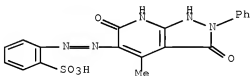
RN 86104-63-4 HCAPLUS

CN Benzenesulfonic acid, 4-[1,3,6,7-tetrahydro-4-methyl-3,6-dioxo-5-(phenylazo)-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)



RN 86104-89-4 HCAPLUS

CN Benzenesulfonic acid, 2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



IT 86104-46-3F 86104-47-4F 86104-49-5F

86104-49-6F 86104-51-0F 86104-59-8F

86104-62-3F 86104-64-5F 86104-65-6F

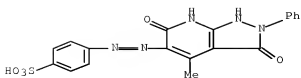
86104-69-0F 86104-71-4F 86104-74-7F

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(dye, manufacture of)

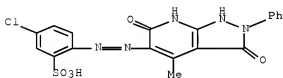
RN 86104-46-3 HCAPLUS

CN Benzenesulfonic acid, 4-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



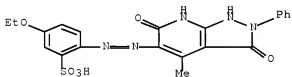
RN 86104-47-4 HCAPLUS

CN Benzenesulfonic acid, 5-chloro-2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



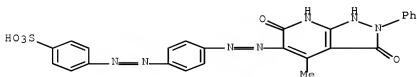
RN 86104-48-5 HCAPLUS

CN Benzenesulfonic acid, 5-ethoxy-2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



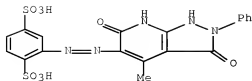
RN 86104-49-6 HCAPLUS

CN Benzenesulfonic acid, 4-[[4-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]phenyl]azo]- (9CI) (CA INDEX NAME)



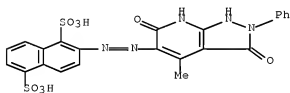
RN 86104-51-0 HCAPLUS

CN 1,4-Benzenedisulfonic acid, 2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



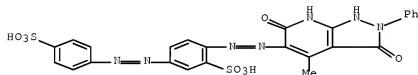
RN 86104-59-8 HCAPLUS

CN 1,5-Naphthalenedisulfonic acid, 2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



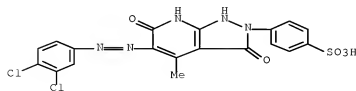
RN 86104-62-3 HCAPLUS

CN Benzenesulfonic acid, 5-[(4-sulphophenyl)azo]-2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



RN 86104-64-5 HCAPLUS

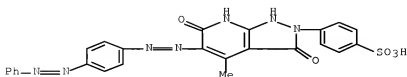
CN Benzenesulfonic acid, 4-[5-[(3,4-dichlorophenyl)azo]-1,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)



RN 86104-65-6 HCAPLUS

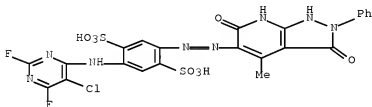
CN Benzenesulfonic acid, 4-[1,3,6,7-tetrahydro-4-methyl-3,6-dioxo-5-[[4-

(phenylazo)phenyl]azo]-2H-pyrazolo[3,4-b]pyridin-2-yl]- (9CI) (CA INDEX NAME)



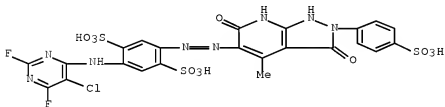
RN 86104-69-0 HCAPLUS

CN 1,4-Benzenedisulfonic acid, 2-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]-5-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



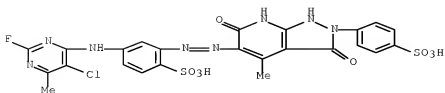
RN 86104-71-4 HCAPLUS

CN 1,4-Benzenedisulfonic acid, 2-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]-5-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-(4-sulfophenyl)-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



RN 86104-74-7 HCAPLUS

CN Benzenesulfonic acid, 4-[(5-chloro-2-fluoro-6-methyl-4-pyrimidinyl)amino]-2-[(2,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2-(4-sulfophenyl)-1H-pyrazolo[3,4-b]pyridin-5-yl)azo]- (9CI) (CA INDEX NAME)



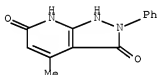
IT 71290-90-7F 86104-35-0P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coupling of, with diazotized aniline derivs.)

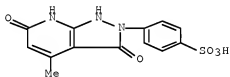
RN 71290-80-7 HCAPLUS

CN 1H-Pyrazolo[3,4-b]pyridine-3,6(2H,7H)-dione, 4-methyl-2-phenyl- (CA INDEX NAME)



RN 86104-85-0 HCAPLUS

CN Benzenesulfonic acid, 4-(1,3,6,7-tetrahydro-4-methyl-3,6-dioxo-2H-pyrazolo[3,4-b]pyridin-2-yl)- (CA INDEX NAME)



L41 ANSWER 73 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1983:143069 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 98:143069

ORIGINAL REFERENCE NO.: 98:21785a,21788a

TITLE: Behavior of β -(4-chloro-3-methylbenzoyl)acrylic acid towards carbon nucleophiles under Michael reaction conditions

AUTHOR(S): El-Hashash, M. A.; Mohamed, M. M.; Islam, I. E.; Abo-Baker, O. A.

CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

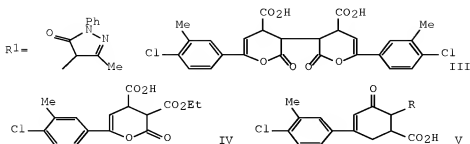
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980), 21B(8), 735-9

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 98:143069
 ED Entered STN: 12 May 1984
 GI



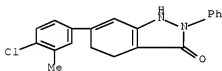
AB Treating 4,3-Cl(Me)C₆H₃COCH:CHCO₂H (I) with active methylene compds., e.g., cyclohexanone, cyclopentanone, camphor, R₁H and EtO₂CCH₂CN in alc. NaOH at 40° gave Michael adducts 4,3-Cl(Me)C₆H₃COCH₂CHRCO₂H (II; R = 2-oxocyclohexyl, 2-oxocyclopentyl, 3-camphoryl, R₁); using EtO₂CCH₂COME and EtO₂CCH₂Ph in boiling alc. NaOH gave II (R = CH₂COME, CH₂Ph). I on treatment with (EtO₂CCH₂)₂ in the presence of NaOMe at room temperature gave III. Fusing III with (EtO₂C)CH₂, MeCOEt, or CH₂(COME)₂, resp., in NaOMe gave IV, V (R = Me, CO₂Et) and an oily CH₂(COME)₂ product whose hydrolysis with 10% KOH gave V (R = H).

IT 94797-23-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and Diels-Alder reaction of)

RN 84797-23-9 HCAPLUS

CN 3H-Indazol-3-one, 6-(4-chloro-3-methylphenyl)-1,2,4,5-tetrahydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 74 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:561974 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 97:161974

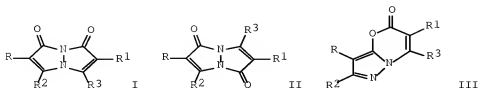
ORIGINAL REFERENCE NO.: 97:27005a,27008a

TITLE: Bimanes. 15. Kinetics and mechanism of the hydroxide ion reaction with 1,5-diazabicyclo[3.3.0]octadienediones (9,10-dioxabimanes)

AUTHOR(S): Kanety, Hannah; Kosower, Edward M.
 CORPORATE SOURCE: Dep. Chem., Tel-Aviv Univ., Tel-Aviv, 69978, Israel
 SOURCE: Journal of Organic Chemistry (1982), 47(22), 4222-6

CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal

LANGUAGE: English
 ED Entered STN: 12 May 1984
 GI



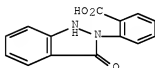
AB The rate consts. for the ring cleavage of I ($R = R_1 = \text{Me}$, H ; $R_2 = R_3 = \text{Cl}$, H) or II ($R = R_1 = \text{Me}$, H ; $R_2 = R_3 = \text{Cl}$, H) have LFER with $[\sigma(R) + 0.5\sigma(R_1)]$ or $[\sigma(R_2) + 0.5\sigma(R_3)]$; ρ is 3.0 or .apprx.4, resp. The ρ for the hydrolysis of III (formed from the photoisomerization of II) is 3.7. The hydrolysis of II or III leads to the name product, the corresponding 1-pyrazolinonylacrylic acids (IV); the hydrolysis of I gives the corresponding 2-pyrazolinonylacrylic acids (V). IV and electrophilic agents gives the corresponding II (predominant) and III; V under similar conditions gives I. ^1H NMR indicates that hydrolysis of I ($R = R_1 = R_2 = R_3 = H$) gives the corresponding (E)-V.

IT 18428-31-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (ring closure of, by electrophilic reagents)

RN 18428-91-6 HCAPLUS

CN Benzoic acid, 2-(1,3-dihydro-3-oxo-2H-indazol-2-yl)- (CA INDEX NAME)



L41 ANSWER 75 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:68404 HCAPLUS Full-text

DOCUMENT NUMBER: 96:68404

ORIGINAL REFERENCE NO.: 96:11233a,11236a

TITLE: Bromination of cyclohexanone-2-carboxamide

AUTHOR(S): Bischoff, Christian; Schroeder, Edith

CORPORATE SOURCE: Zentralinst. Org. Chem., DAW, Berlin-Adlershof,
 DDR-1199, Ger. Dem. Rep.

SOURCE: Journal fuer Praktische Chemie (Leipzig) (1981
), 323(4), 616-20

CODEN: JPCEAO; ISSN: 0021-8383

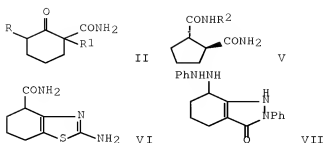
DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 96:68404

ED Entered STN: 12 May 1984

GI



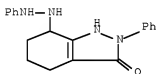
AB Brominating the title compound (I) in the presence of Na₂CO₃ gave II (R = H, R₁ = Br) (III), but II (R = Br, R₁ = H) (IV) without Na₂CO₃. Favorskii rearrangement of III with R₂NH₂ [R₂ = H, Pr, Bu, Me(CH₂)₅, 4-ClC₆H₄] or piperidine gave the corresponding V. Cyclocondensation of IV and H₂NC(S)NH₂ gave VI. Treating III with pyridine gave a salt which was treated with PhNNH₂ to give VII.

IT 80193-15-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 80193-15-3 HCAPLUS

CN 3H-Indazol-3-one, 1,2,4,5,6,7-hexahydro-2-phenyl-7-(2-phenylhydrazino)-
(9CI) (CA INDEX NAME)



'L999-L998' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'

The following are valid formats:

ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data

IPC ----- International Patent Classifications
 MAX ----- ALL, plus Patent FAM, RE
 PATS ----- PI, SO
 SAM ----- CC, SX, TI, ST, IT
 SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
 SCAN must be entered on the same line as the DISPLAY,
 e.g., D SCAN or DISPLAY SCAN)
 STD ----- BIB, CLASS

 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IMAX ----- MAX, indented with text labels
 ISTD ----- STD, indented with text labels

 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 HIT ----- Fields containing hit terms
 HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
 containing hit terms
 HITRN ----- HIT RN and its text modification
 HITSTR ----- HIT RN, its text modification, its CA index name, and
 its structure diagram
 HITSEQ ----- HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 FHITSTR ----- First HIT RN, its text modification, its CA index name, and
 its structure diagram
 FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 KWIC ----- Hit term plus 20 words on either side
 OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
 ENTER DISPLAY FORMAT (BIB):END

=> D IBIB ED ABS HITSTR 117-133 L41

L41 ANSWER 117 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1960:34230 HCAPLUS Full-text
 DOCUMENT NUMBER: 54:34230
 ORIGINAL REFERENCE NO.: 54:6699h-i,6700a-d
 TITLE: Heterocycles. IX. Resonance effects in
 pyrazolin-5-ones and related compounds
 AUTHOR(S): DeStevens, George; Halamandaris, Angela; Wenk,
 Patricia; Dorfman, Louis
 CORPORATE SOURCE: Ciba Pharm. Products, Inc., Summit, NJ
 SOURCE: Journal of the American Chemical Society (1959)

), 81, 6292-5
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 54:34230

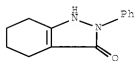
ED Entered SIN: 22 Apr 2001

AB cf. C.A. 54, 1528g. The spectral properties of tetrahydroindazolone, structurally related to pyrazolin-5-one, suggested that this type of compound existed predominantly in the dipolar zwitterion form; the predominance of this structure was demonstrated by several chemical reactions. 2-Hydrazino-3-methyl-5,6,7,8-tetrahydroquinazolin-4-one (6 g.) and 15 cc. N2H4.H2O in 25 cc. EtOH refluxed 4 hrs., cooled, and acidified with glacial AcOH gave 1.2 g. 4,5,6,7-tetrahydro-3(1)-indazolone (I), m. 298-300°. Et 2-oxocyclopentanecarboxylate (5.25 g.) and 15 cc. N2H4.H2O heated 3 hrs. at 125° and cooled gave 1.0 g. 2-hydrazino-2-hydroxycyclopentanecarbohydrazide, m. 184-5° (EtOH). Et 2-oxocyclohexanecarboxylate (3.4 g.), 10 cc. N2H4.H2O, and 30 cc. EtOH refluxed 2 hrs., cooled, filtered from I, evaporated in vacuo, and kept several days at room temperature deposited 0.1 g. 2-hydrazino-2-hydroxycyclohexanecarbohydrazide, m. 196-8°. Et 1-benzyl-2-oxocyclohexanecarboxylate (II) (15 g.) and 45 cc. N2H4.H2O refluxed 45 min., cooled, and filtered gave 11 g. 3a-PhCH2 derivative (III) of I, needles, m. 180-2° (EtOH); the mother liquor concentrated to half-volume and cooled overnight gave 1.5 g. 1-benzyl-2-hydrazino-2-hydroxycyclohexanecarbohydrazide, m. 143-4° (EtOH). II (4 g.) and 1.65 g. PhNNH2 heated 2.5 hrs. at 125°, distilled, and the distillate, b0.6 210-14°, tritreated with petr. ether (b. 35-60°) gave 1.3 g. 2-Ph derivative of III, m. 78-80°. Et 1-(β-diethylamino-ethyl)-2-oxocyclohexanecarboxylate (3.5 g.) and 10 cc. N2H4.H2O refluxed 8 hrs. and cooled overnight, the resulting gel dissolved in 50 cc. H2O and extracted with Et2O, and the extract dried and treated with gaseous HBr yielded 1.5 g. 3a-Et2N(CH2)2NH derivative of I.HCl, m. 184-5° (1:1 EtOH-EtOAc). I (3.75 g.) and 2.42 g. 55% NaNH2 in 50 cc. dry PhMe refluxed 5 hrs., treated with 1 equivalent BuBr, refluxed 14 hrs., filtered, and evaporated in vacuo gave 1.3 g. 2-Bu derivative of I, needles, m. 114-15°. CF3COCH2CO2Et (IV) (4 g.) and 1.4 g. N2H4.H2O in 25 cc. EtOH refluxed 2 hrs., evaporated in vacuo, treated with 20 cc. H2O, and acidified with concentrated HCl to pH 3 yielded 2.5 g. 3- trifluoromethylpyrazolin-5-one (V), m. 210-12° (1:1 Et2O-petr. ether). MeNNH2.H2SO4 (5.9 g.) in 10 cc. H2O neutralized with 1 equivalent NaOH, treated with 5.0 g. IV, diluted with 10 cc. H2O, refluxed 2 hrs., cooled, and filtered gave 1.1 g. 1-Me derivative of V, m. 174-5.5° (1:1 Et2O-petr. ether). IV and PhNNH2 heated 4 hrs. at 125° yielded 75% 1-Ph derivative of V, m. 185-7° (aqueous EtOH). 6-Benzyl-2,3,4,4a,5,6,7,8-octahydro-3-cinnoline, m. 137-8°, was prepared by the method of Clarke and Lapworth (C.A. 1, 848). The characteristic infrared frequencies of the various compds. were tabulated.

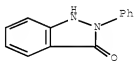
IT 62221-94-7, 3-Indazolinone, 4,5,6,7-tetrahydro-2-phenyl-
 (spectrum of)

RN 62221-94-7 HCAPLUS

CN 3H-Indazol-3-one, 1,2,4,5,6,7-hexahydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 118 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1960:23166 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 54:23166
 ORIGINAL REFERENCE NO.: 54:4607f-i
 TITLE: Studies on the reaction of carbon monoxide under high pressure. IV. Reaction of carbon monoxide and azobenzene
 AUTHOR(S): Horie, I. Shigeki
 CORPORATE SOURCE: Osaka Univ., Sakai
 SOURCE: Nippon Kagaku Zasshi (1958), 79, 499-504
 CODEN: NPKZAZ; ISSN: 0369-5387
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 ED Entered STN: 22 Apr 2001
 AB PhN:NPh (I) (5 g.), 1 g. [Co(CO)₄]₂ (II), and 25 cc. C₆H₆ charged in an autoclave, 150 atmospheric CO added, and the mixture heated 4 hrs. at 180-90° and filtered gave 2-(3-hydroxyindazol-2-yl)benzoic acid lactone (III), m. 296°, and (PhNH)2CO (IV) from the alkali-insol. part. The alkali-soluble part gave 0.8 g. 3-phenyl-2,4-dioxo-1,2,3,4-tetrahydroquinazoline (V), m. 275°, and 2.8 g. 2-phenylindazolone (VI), m. 204°. o-H₂NC₆H₄CONH₂ (8.0 g.) in 100 cc. Ac₂O treated with 6.2 g. PhNO and reduced with Zn and EtOH gave 3.0 g. VI. VI (2 g.), 1.0 g. II, and 50 cc. C₆H₆ treated with 150 atmospheric CO 2 hrs. at 230° gave 1.8 g. V. Similarly, 5 g. I, II, and CO at 220-30° gave III, IV, and 4.5 g. V. Fe(CO)₅, Co acetylacetonate, and Co stearate under similar conditions gave 12.3%, 23.1%, and 29.2% V, resp. V (2.0 g.) in 10 cc. 10% NaOH boiled 2.5 hrs., extracted with Et₂O, and the aqueous layer made up to pH 4.0 gave o-H₂NC₆H₄CO₂H (VII), and 2 g. V with 8 g. KOH in 40 cc. EtOH gave 0.8 g. o-(PhNHCONH)C₆H₄CO₂H (VIII), m. 187-8° (decomposition). VIII was also prepared from VII and PhNCO. Similarly was prepared o-(PhNHCONH)C₆H₄CO₂Et (IX), m. 148°. Heating 1.0 g. VIII 30 min. at 190° gave 0.05 g. V. VIII (1.0 g.) in 30 cc. EtOH treated with dry HCl. gave 0.9 g. V. IX (0.2 g.) heated 3 hrs. at 200° in a sealed tube yielded 0.03 g. V. VII (5.0 g.) and 5.0 g. PhNHCONH₂ heated 5 hrs. at 200° in a sealed tube gave 2.5 g. V.
 IT 17049-65-9F, 3-Indazolinone, 2-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 17049-65-9 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)

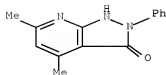


L41 ANSWER 119 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1960:11425 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 54:11425
 ORIGINAL REFERENCE NO.: 54:2323b-h
 TITLE: Synthesis of 2-aminonicotinamides by Raney nickel cleavage of pyrazolo[3,4-b]pyridines
 AUTHOR(S): Taylor, Edward C., Jr.; Barton, J. W.
 CORPORATE SOURCE: Princeton Univ., Princeton, NJ
 SOURCE: Journal of the American Chemical Society (1959), 81, 2448-52
 CODEN: JACSAT; ISSN: 0002-7863

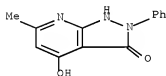
DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 54:11425
 ED Entered STN: 22 Apr 2001

AB Et cyanoacetate (22.6 g.) 10 ml. 98% H₂NNHMe and 200 ml. EtOH refluxed 48 hrs. and chilled 3 hrs. at 0° gave 6.1 g. 1-methyl-3-amino-5-pyrazolone, m. 197-8° (EtOH). Evaporation of the mother liquor over 1 week gave 7 g. 2-methyl-3-amino-5-pyrazolone, m. 180-2°. The pyrazolone (I) (0.2 mole) in 20 ml. 5% NaOH stirred and treated 1 hr. at 40-50° with 0.3 mole 1,3-diketone, the mixture adjusted to pH 5 with AcOH and cooled to 0° gave the pyrazolo[3,4-b]pyridine (II). II (10 g.), 100 g. Raney Ni and 1 l. EtOH stirred 3 hrs. at reflux, filtered and extracted with hot EtOH and the combined filtrates dried in vacuo gave the 2-aminonicotinamide (III). 4-Methoxymethyl-6-methyl derivative (IIIa) III of (0.5 g.) and 20 ml. 50% H₂SO₄ refluxed 3 hrs., poured over ice, and NH₄OH added to pH 4-5 gave 0.38 g. lactone of 2-amino-4-hydroxymethyl-6-methylnicotinic acid, m. 253-4° (EtOH). The lactone of 2-hydroxy-4-hydroxymethyl-6-methylnicotinic acid (0.41 g.), m. 332-4° (decomposition), was obtained by refluxing 1 g. IIIa and 40 ml. 50% H₂SO₄ 3 hrs., cooling, adding to 100 ml. H₂O, cooling to 0° and treating with 0.4 g. NaNO₂ in 5 ml. H₂O, and warming 15 min. at 80°. 2-Anilino-4-methoxymethyl-6-methylnicotinamide (1 g.) treated with 40 ml. 50% H₂SO₄ as above gave 0.54 g. lactone of 2-anilino-4-hydroxymethyl-6-methylnicotinic acid, m. 151-2°. 3-Amino-5-pyrazolone (IVa) (10 g.), 20 ml. MeCOCH₂CO₂Et (IV), and 100 ml. 5% NaOH stirred 1 hr. at 50-60°, 100 ml. H₂O and AcOH (to pH 5) added gave the 3,4-dihydroxy-6-methyl derivative of II (quant.), m. 356-8° (decomposition) (HeONMe₂); monoacetyl derivative m. 255-6° (decomposition). Alternatively, IVa, 35 ml. IV, and 100 ml. glacial AcOH was refluxed 45 min. cooled, the solid mass ground with EtOH and filtered to give after repetition of this process, 27.6 g. powder which on acetylation gave 3,4-dihydroxy-6-methyl derivative (V) of II acetyl derivative, m. 254-6°. Evaporation of filtrate and extraction with boiling EtOH left a powder, m. 325-7° (EtOH), an isomeric acetyl derivative. Cooling the EtOH extract yielded the diacetyl derivative, decompose above 260°, which gives the monoacetyl derivative, m. 325-7°, on prolonged boiling in EtOH. Hydrolysis of the monoacetyl (m. 325-7°) or diacetyl derivs. with 10% NaOH followed by acidification with AcOH gave the 3,6-dihydroxy-4-methyl derivative (Va) of II. V(10 g.), 100 g. Raney Ni and 1 l. EtOH refluxed 3 hrs., filtered, extracted with EtOH and the filtrates dried yielded 2.1 g. 4-hydroxy-6-methyl derivative of III, m. 242-3° (no color with ethanolic FeCl₃). Similarly, 10 g. Va yielded 3.3 g. 4-methyl-6-hydroxy derivative of II, m. 249.51° (H₂O), red-brown color with ethanolic FeCl₃. 1-Phenyl-3-amino-5-pyrazolone (VI) (8.75 g.), 10 ml. IV, and 50 ml. AcOH refluxed 45 min., cooled and diluted with an equal volume of EtOH gave 9.6 g. condensation product, m. 306-8° (decomposition). Alternatively, 4.4 g. VI, 4 ml. IV, and 50 ml. EtOH containing 0.5 g. Na was refluxed and stirred 1 hr., cooled, diluted with Et₂O and filtered, the solid dissolved in 50 ml. H₂O and the pH adjusted to 4-5 with AcOH to give 3.4 g. of the same product, m. 307° (decomposition); Ac derivative m. 145-6°.

IT 71290-77-2P, 3H-Pyrazolo[3,4-b]pyridin-3-one, 1,2-dihydro-4,6-dimethyl-2-phenyl- 109103-52-8P, 3H-Pyrazolo[3,4-b]pyridin-3-one, 1,2-dihydro-4-hydroxy-6-methyl-2-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 71290-77-2 HCAPLUS
 CN 3H-Pyrazolo[3,4-b]pyridin-3-one, 1,2-dihydro-4,6-dimethyl-2-phenyl- (CA
 INDEX NAME)



RN 109103-52-8 HCAPLUS

CN 3H-Pyrazolo[3,4-b]pyridin-3-one, 1,2-dihydro-4-hydroxy-6-methyl-2-phenyl-
(CA INDEX NAME)

L41 ANSWER 120 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1960:1824 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 54:1824

ORIGINAL REFERENCE NO.: 54:336h-i,337a-d

TITLE: Dieckmann reaction. VI. Cyclization of the diethyl ester of α -acetyl- and α -benzoylpimelic acid

AUTHOR(S): Zaretskii, V. I.; Vul'fson, N. S.

CORPORATE SOURCE: Sci. Research Inst. Org. Intermediates and Dyes, Moscow

SOURCE: Zhurnal Obshchei Khimii (1959), 29, 416-21

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB cf. C.A. 53, 1177g. To NaHCO₂Et, from 65 g. ester, 5.75 g. Na, and 100 ml. absolute EtOH, there was added 41.2 g. Et δ -chlorovalerate at 10-15°, along with 19.7 g. NaI. and the mixture was refluxed 20 hrs.; after concentration, addition of H₂O, acidification with H₂SO₄, and extraction with C₆H₆ there was obtained by distillation of the washed organic extract 74.4-6.6% di-Et α -acetylpyimelate (I), b_{2.5} 141-6°, n_{20D} 1.4445, d₂₀ 1.0430. The use of Et δ -bromovalerate resulted in a 60% yield. Similarly, BzCHNaCO₂Et, from 96 g. ester and 41.2 g. Et δ -chlorovalerate, and 19.7 g. NaI gave, in 14.5 hrs. of refluxing, followed by addition of 8 g. NaI and refluxing 13 hrs. longer, 81.5% di-Et α -benzoylpimelate (II), b_{1.5} 193-4.5°, 1.5000, 1.0900. To 4.7 g. powdered Na in xylene there was rapidly added 38.7 g. I, the mixture was stirred until the exothermic reaction had ceased, then was refluxed with stirring 5-6 hrs., freed of EtOAc by distillation, the residue treated with ice at -5° acidified to Congo red with HCl and extracted with xylene or C₆H₆; the washed extract gave 52.2-2.5% 2-carbethoxycyclohexanone (III), b_{2.5} 71.5-75°, 1.4780, 1.0675; the results were similar if the reaction was run with addition of 2-3 drops absolute EtOH or in the presence of EtONa which had been freed of EtOH; in the latter case the yield was 55.7%. Heating the product with PhNHNH₂ gave 90.7% 2-phenyl-4,5,6,7-tetrahydro-3-indazolone, m.p. 179-80°.

Similar reaction of 25.8 g. I in the presence of but 2.1 g. powdered Na gave only a 16% yield of III, along with 13.9% EtO2C(CH2)5CO2Et. To a solution of EtONa, from 4.5 g. Na and 100 ml. absolute EtOH, there was added 33.5 g. I and the whole was refluxed 3 hrs., concentrated to remove EtOH, treated with ice, acidified with dilute H2SO4, and extracted with Et2O to yield 34.7% EtO2C(CH2)5CO2Et and 2.9 g. III. Similar cyclization of 48 g. II with 4.7 g. Na in xylene gave 14.8 g. crude product which, after extraction with 6% KOH, gave 2.9 g. EtOBz and some 55% unisolated III. Refluxing III with EtONa in EtOH 3 hrs. gave mainly unreacted III and 3.1% EtO2C(CH2)5CO2Et. Similar treatment of I gave 22% yield, and the use of equimolar amount of EtONa gave a 56% yield. Refluxing I with powdered Na in xylene in the presence of absolute EtOH 5.5 hrs. gave 49% EtO2C(CH2)5CO2Et. Hydrolysis of di-Et α -carbethoxypimelate and esterification of the free acid with EtOH gave 76.7% EtO2C(CH2)5CO2Et, b3 104-6°, 1.4295, 0.9928; dihydrazide m. 185-5.5°. This (21.6 g.) cyclized by 3 hrs. refluxing with 3.5 g. Na dissolved in absolute EtOH gave 5.8% III and unchanged starting material. Similar cyclization run in xylene with dry EtONa gave 57.6% III.

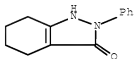
IT 62221-94-7P, 3-Indazolinone, 4,5,6,7-tetrahydro-2-phenyl-

RL: PREP (Preparation)

(preparation of)

RN 62221-94-7 HCAPLUS

CN 3H-Indazol-3-one, 1,2,4,5,6,7-hexahydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 121 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1959:6630 HCAPLUS Full-text

DOCUMENT NUMBER: 53:6630

ORIGINAL REFERENCE NO.: 53:1177f-i,1178a-b

TITLE: Dieckman reaction. V. Cyclization of diethyl ester of α -carbethoxypimelic acid

AUTHOR(S): Vul'fson, N. S.; Zaretskii, V. I.

CORPORATE SOURCE: K. E. Voroshilov Sci. Research Inst. Org. Intermed. and Dyes, Moscow

SOURCE: Zhurnal Obshchei Khimii (1958), 28, 1909-14

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

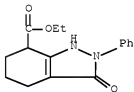
OTHER SOURCE(S): CASREACT 53:6630

ED Entered STN: 22 Apr 2001

AB cf. C.A. 52, 13658b. Mono-Et adipate was prepared according to Swann, et al. (Synthesis of Organic Preparations, 1949, volume II, p. 345), 61.8%, b2 129-32.5°, m. 27.4°. This was converted to Et δ -bromovalerate (I), 88.7%, b2 71°, n20D 1.4605, d20 1.3085 (cf. Jilek and Michajlyszyn, C.A. 49, 9507e). Hydrolysis of 1,1,1,5-tetrachloropentane gave 52.5% δ -chlorovaleric acid, b2.5 101.5°, b2 101.5°, m. 18.25°, n20D 1.4545, d20 1.1644, which with EtOH and H2SO4 in C6H6 gave 86% Et δ -chlorovalerate (II), b1.5 53°, b1 52.5°, n20D 1.4305, d20 1.0518. I with NaCH(CO2Et)2 in hot EtOH gave 75.5% di-Et α -carbethoxypimelate (III), b2 146.5-50°, n20D 1.4380, d20 1.0561; from II the yield was 83%. III (43.2 g.) and 0.3 ml. dry EtOH was added to 4.7 g. powdered Na in xylene and after stirring 10 min. the mixture was refluxed 5-6

hrs. yielding after an aqueous treatment 57% 2,6-dicarbethoxycyclohexanone (IV), b12 165-75°, n18.5D 1.4692, d18.5 1.1239; with PhNHNH2 it gave 86% 1-phenyl-3,4,1',2'-tetrahydrobenzo-3-carbethoxypyrazol-5-one, m. 151-1.5°. IV (17 g.) in 34 ml. dry MeOH was treated with 12 ml. MeI, then at -15°, with MeONa from 3.5 g. Na, and kept overnight at 0°; after refluxing until neutral, the mixture was concentrated, treated with H2O, and extracted with Et2O yielding 75% 2,6-dimethyl-2,6-dicarbethoxycyclohexanone (V), b2 113-16°, n20D 1.4620-1.4625; to sep. a trace of unmethylated product V was treated with cold 15% KOH and H2O, yielding a pure product, b3 123.5-6.5°, n20D 1.4615, d20 1.086. This kept 12 days with MeOH-KOH gave after an aqueous treatment, extraction with Et2O, and acidification of the aqueous solution followed by steam distillation 50.5% 2,6-dimethylcyclohexanone, b743 167-70.5°, n20D 1.4475-1.4480, d20 0.9087; semicarbazone, m. 181-2°. IV (18.2 g.) in 34 ml. MeOH was treated with 6.5 ml. MeI and MeONa from 1.9 g. Na yielding after 24 hrs. near 0° 72.8% 2-methyl-2,6-dicarbethoxycyclohexanone, b1 112-14°, n20D 1.4645-1.4655, d20 1.0986 (a violet color with FeCl3); this decarboxylated as above yielded 37.3% 2-methylcyclohexanone, b730 162.5-6°, n20D 1.4485, d20 0.9224; semicarbazone, m. 188.5-9°.

IT 101289-05-8P, 7-Indazolinecarboxylic acid, 4,5,6,7-tetrahydro-3-oxo-2-phenyl-, ethyl ester
 RL: PREP (Preparation)
 (preparation of)
 RN 101289-05-8 HCAPLUS
 CN 7-Indazolinecarboxylic acid, 4,5,6,7-tetrahydro-3-oxo-2-phenyl-, ethyl ester (6CI) (CA INDEX NAME)



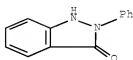
L41 ANSWER 122 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1958:82938 HCAPLUS
 DOCUMENT NUMBER: 52:82938
 ORIGINAL REFERENCE NO.: 52:14701a
 TITLE: 3-Indazolone
 INVENTOR(S): Murahashi, Shunsuke; Horie, Shigeki
 PATENT ASSIGNEE(S): Osaka University
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------|
| JP 32008925 | B4 | 19571019 | JP | <-- |
| ED Entered STN: 22 Apr 2001 | | | | |
| AB PhN:NPh (5 g.) in 20 ml. C6H6 and 1 g. [Co(CO)4]2 in an autoclave with CO at 100 atmospheric heated 2 hrs. at 190-200°, the product distilled, the distillate taken up in 2% NaOH and acidified with HCl gave 3.2 g. 2-phenyl-3-indazolone, needles, m. 204°. | | | | |
| IT 101289-05-8P, 3-Indazolinone, 2-phenyl- | | | | |

RL: PREP (Preparation)
(preparation of)

RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 123 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:55949 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 52:55949

ORIGINAL REFERENCE NO.: 52:10106g-i,10107a-i,10108a-i

TITLE: Pteridines. XVI. A synthesis of 2-aminopyrazine-3-

carboxamides by reductive ring cleavage of

3-hydroxy-1-pyrazolo[b]pyrazines

Taylor, E. C., Jr.; Barton, J. W.; Osdene, T. S.

Princeton Univ., Princeton, NJ

SOURCE: Journal of the American Chemical Society (1958

), 80, 421-7

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:55949

ED Entered STN: 22 Apr 2001

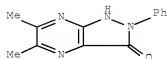
AB cf. C.A. 50, 13047b. PhN:NCH(CN)CO₂Et (I) (4.1 g.) and 25 cc. EtOH refluxed 15 min. with 1.4 g. N₂H₄·H₂O, cooled to 0°, and filtered yielded 3.6 g. 3-hydroxy-4-phenylazo-5-aminopyrazole (II), deep red needles, m. 256° (decomposition). HON:C(CN)CONHNH₂ N₂H₄ salt (III) (5.0 g.) in 25 cc. 40% aqueous NaOH kept 1 hr. at 60°, acidified with glacial AcOH, and filtered gave 3.87 g. 3-hydroxy-4-nitroso-5-aminopyrazole (IV); a similar run heated 0.5 hr. on the steam bath gave 2.56 g. IV. III (5.0 g.) in 100 cc. EtOH containing 6 g. Na refluxed 4 hrs. with stirring and filtered, and the residue dissolved in 25 cc. H₂O, acidified with glacial AcOH, and cooled gave 4.0 g. IV. II (4.0 g.) in 50 cc. 98% HCO₂H hydrogenated at 3 atmospheric over 0.4 g. 10% Pd-C, filtered, and evaporated, the residue triturated with 1:1 EtOH-Et₂O, and the undissolved material recrystd. with C from H₂O gave 2.95 g. diformyl derivative (V) of 3-hydroxy-4,5-diaminopyrazole (VI), m. 212-13° (decomposition). IV (2.0 g.) in 40 cc. 98% HCO₂H hydrogenated over 10% Pd-C yielded 2.05 g. V. V (8 g.) in 30 cc. 50% H₂SO₄ warmed to beginning crystallization, diluted with boiling H₂O to solution, and cooled slowly yielded 9.4 g. VI·H₂SO₄, light yellow crystals. I (32.5 g.), 7.5 cc. 99% MeNHNH₂, and 250 cc. EtOH refluxed 4 hrs. and cooled to 0° gave 27 g. 1-Me derivative (VII) of II, m. 265° (EtOH). HON:C(CN)CO₂Et (7.1 g.), 5 cc. 99% MeNHNH₂, and 30 cc. EtOH refluxed 3 hrs., refluxed 1 hr. with stirring with 30 cc. 30% alc. KOH, cooled to 0°, and filtered, and the residue dissolved in 20 cc. H₂O and adjusted with AcOH to pH 5 yielded 2.9 g. 1-Me derivative (VIII) of IV, m. 184-6°; 2nd crop, 0.3 g. VII (20 g.) in 100 cc. 90% HCO₂H hydrogenated 45 min. at 3 atmospheric over 1 g. 10% Pd-C, filtered, and evaporated in vacuo, the residual oil washed with Et₂O and dissolved in 70 cc. EtOH, and the solution cooled gave 12.8 g. monoformyl derivative (IX) of the 1-Me derivative (X) of VI, m. 210°; it gave recrystd. from aqueous EtOH a lower-melting hydrate, m. 188-9° with loss of moisture at 133-5°. VIII (2.0 g.) in 40 cc. 90% HCO₂H hydrogenated in the usual manner and evaporated in

vacuo, and the residual brown oil dissolved in a small amount of EtOH and cooled at 0° yielded 1.5 g. IX, m. 188-90°. IX (10 g.) recrystd. from 30 cc. 20% H2SO4 containing 25 cc. EtOH yielded 13.9 g. X.H2SO4, m. above 300°. 1-Phenyl-3-hydroxy-5-aminopyrazole (5.25 g.) in 50 cc. 10% aqueous NaOH added dropwise to PhN2Cl in NaOAc buffer (from 3 g. PhNH2, 6 cc. concentrated HCl, 2.1 g. NaNO2, and 12 cc. H2O) stirred 0.5 hr., and filtered gave 7.95 g. 1-Ph derivative (XI) of II, deep yellow plates, m. 266-8° (decomposition) (Cellosolve). 2-Phenyl-3-hydroxy-5-aminopyrazole yielded similarly 91% 2-Ph derivative (XII) of II, purple-red needles, m. 194-5° (EtOH). I (40 g.), 20 cc. PhNHNH2, and 200 cc. iso-AmOH refluxed 24 hrs., cooled to room temperature, and filtered, and the residue washed with 100 cc. cold EtOH gave 24.2 g. XII; the mother liquor kept at 0° overnight deposited 1.8 g. phenylazomalonalanamide phenylhydrazine N-phenylhydrazide, yellow needles, m. 187-8° (EtOH). I (4 g.) and 2 cc. PhNHNH2 refluxed 20 hrs. with 0.87 g. Na in 75 cc. iso-AmOH and evaporated in vacuo, the residue triturated with 50% aqueous AcOH, the resulting solid extracted with 200 cc. boiling EtOH, and the extract concentrated to 50 cc. and cooled yielded 1.39 g. XII; the EtOH-insol. residue recrystd. from Cellosolve yielded 0.82 g. XI, m. 266-8° (decomposition). XI (5.0 g.) in 50 cc. 90% HCO2H hydrogenated 1 hr. at room temperature and 3 atmospheric over 0.5 g. 10% Pd-C, filtered, and evaporated in vacuo, and the oily residue triturated with 50 cc. 1:3 EtOH-Et2O gave 3.1 g. monoformyl derivative (XIII) of 1-phenyl-3-hydroxy-4,5-diaminopyrazole (XIV), plates, m. 223-5° (decomposition) (aqueous EtOH). Crude XIII (3.1 g.) warmed on a water bath with 3 cc. concentrated H2SO4, 7 cc. H2O, and 3 cc. EtOH, diluted with 4 cc. EtOH, and cooled gave 4.8 g. XIV.H2SO4, yellow needles. XII (8.0 g.), 100 cc. 90% HCO2H, and 0.8 g. 10% Pd-C hydrogenated at 3 atmospheric yielded 4.8 g. monoformyl derivative (XV) of 2-phenyl-3-hydroxy-4,5-diaminopyrazole (XVI), m. 235° (decomposition) (aqueous EtOH). XII (12 g.) converted to the XV and the crude product crystallized from 1:1 30% H2SO4-EtOH yielded 11.6 g. XVI.H2SO4, orange plates. VI.H2SO4 (20 g.) and 28 g. glyoxal-NaHSO3 adduct (XVII) in 250 cc. H2O treated dropwise with stirring at 60°, stirred 0.5 hr., adjusted to pH 5, cooled to 0°, and filtered gave 9.9 g. 3-hydroxy-1-pyrazolo[b]pyrazine (XVIII), yellow, m. 314-15° (decomposition). VI.H2SO4 (1.5 g.) in 10 cc. H2O treated with shaking with 1 cc. Ac2 and filtered yielded 0.93 g. 5,6-di-Me derivative (XIX) of XVIII, yellow, m. 325° (decomposition) (sublimed at 230°/0.1 mm.). VI.H2SO4 (4.2 g.), 6.3 g. Bz2, 1.2 g. NaOH, 30 cc. EtCOMe, 30 cc. EtOH, and 20 cc. H2O refluxed 1.5 hrs., concentrated in vacuo to about 1/6 its original volume, basified with aqueous NaOH, treated with C, and filtered, the filtrate acidified with HCl, and the precipitate repptd. from aqueous NaOH with HCl and dried azeotropically with C6H6 yielded 3.5 g. 5,6-di-Ph derivative (XX) of XVIII, yellow, m. 269° (decomposition) (EtOAc). X.H2SO4 (4.52 g.), 5.6 g. XVII, and 40 cc. H2O adjusted slowly with stirring to pH 5, kept at room temperature overnight, and filtered gave 2.84 g. 1-Me derivative (XXI) of XVIII, bright yellow needles, m. 242-3° (sublimed at 200°/0.1 mm.). XVIII (1.0 g.) in 10 cc. 10% aqueous NaOH treated at 60° with stirring with 1.4 g. MeI and evaporated in vacuo after 45 min., and the residue dissolved in a little H2O and repptd. with AcOH (pH 5) yielded 0.62 g. XXI. X.H2SO4 (1.13 g.), 0.5 cc. Ac2, and 10 cc. H2O treated dropwise with NH4OH to pH 7-8 and readjusted to pH 5 after 10 min. with AcOH gave 0.78 g. 1,5,6-tri-Me derivative of XVIII, m. 268-9° (EtOH and sublimed at 200°/0.1 mm.). X.H2SO4 (1.0 g.), 1 g. Bz2, 10 cc. H2O, 10 cc. EtAc, and 10 cc. EtOH adjusted to pH 8 with 40% aqueous NaOH, refluxed 1.5 hrs., kept at room temperature overnight, and concentrated in vacuo, the residue diluted with H2O, the suspension adjusted with NaOH to pH 9, and the solution heated to boiling, treated with C, filtered, and acidified with AcOH yielded 0.35 g. 1-Me derivative of XX, m. 258-60° (EtOH and sublimed at 200°/0.1 mm.). XVIII (15 g.) in 150 cc. 10% aqueous NaOH and 15 cc. EtOH treated with 15 cc. PhCH2Cl, evaporated after 1 hr. in vacuo, acidified with 50% aqueous AcOH, and filtered gave 18.4 g. 1-PhCH2 derivative (XXII) of XVIII, pale yellow needles, m. 175-6° (MeOH). XIV.H2SO4 (12 g.) and 13 g. XVII in 150 cc. H2O adjusted

slowly with concentrated NH₄OH to pH 7-8, stirred 45 min., readjusted to pH 5 with glacial AcOH, and cooled to 0° yielded 7.7 g. 1-Ph derivative (XXIII) of XVIII, lime-green needles, m. 227-9° (aqueous EtOH). XVI.H₂SO₄ (37 g.), 40 g. XVII, and 400 cc. H₂O gave in the same manner 23.2 g. 2-phenyl-1-pyrazolo[b]pyrazin-3(2H)-one (XXIV), pale green plates, m. 232-3.5° (EtOH). XVI.H₂SO₄ (0.96 g.), 0.4 cc. Ac₂, and 100 cc. H₂O yielded in the same manner 0.8 g. 5,6-di-Me derivative of XXIV, m. 239-40°, which recrystd. from EtOH and sublimed at 200°/0.1 mm. gave another polymorphic form, m. 193-5°. VI.H₂SO₄ (8.5 g.) and 8.8 g. NaHSO₃ in 100 cc. H₂O treated with 6 cc. 47.5% AcCHO, treated dropwise with stirring at 60° until the pH reached 7-8, stirred 45 min., adjusted with dilute AcOH to pH 4-5, and cooled to 0° gave 3.83 g. 6-Me derivative (XXV) of XVIII, light yellow needles, m. 319-21° (H₂O); the mother concentrated in vacuo to 1/3 the original volume and kept 24 hrs. at 0° gave 1.15 g. 5-Me derivative (XXVI) of XVIII, buff-colored prisms, m. 234-5° (EtOH). XVIII (1.0 g.), 20 cc. HCONH₂, and 3 g. Raney Ni heated 1.5 hrs. with stirring at 115-20°, treated with an addnl. 2 g. catalyst, heated again 1.5 hrs. with stirring, filtered, and cooled yielded 0.58 g. 2-aminopyrazine-3-carboxamide (XXVII), m. 244-5°. XIX (0.5 g.), 50 cc. 95% EtOH, and 6 g. Raney Ni refluxed 2 hrs., filtered, and evaporated, and the solid residue sublimed at 200°/0.1 mm. gave 0.28 g. 5,6-di-Me derivative (XXVIII) of XXVII, light yellow, m. 255°. IV (1.28 g.) in 40 cc. H₂O containing 2 cc. concentrated NH₄OH refluxed 7 hrs. with 1.2 g. Ac₂ and 4 g. Raney Ni, filtered, and cooled to 0° gave 0.32 g. XXVIII; the Raney Ni residue extracted with boiling EtOH gave an addnl. 0.06 g. XXVIII. XX (1.0 g.), 50 cc. 95% EtOH, and 8 g. Raney Ni refluxed 3 hrs., filtered, and evaporated in vacuo, the residue triturated with H₂O and filtered, and the insol. portion washed, dried (0.8 g.), and sublimed at 190°/0.01 mm. yielded the 5,6-di-Ph derivative of XXVII, bright yellow, m. 203-5°. XXI (1.0 g.), 100 cc. 95% EtOH, and 5 g. Raney Ni refluxed 2.5 hrs., filtered, and evaporated in vacuo gave 0.38 g. 2-MeNH analog of XXVII, light yellow rods, m. 200-1° (sublimed at 180°/0.1 mm.). XXIII (6 g.), 60 g. Raney Ni, and 600 cc. EtOH refluxed 4 hrs. with stirring and filtered through Celite, the filter cake extracted with hot EtOH, the combined filtrate and washing evaporated in vacuo, and the residue (3.2 g.) recrystd. gave the 2-PhNH analog of XXVII, greenish yellow plates from EtOH by slow crystallization or needles by rapid cooling, m. 175-6°. XXIV (5.0 g.), 500 cc. 95% EtOH, and 50 g. Raney Ni refluxed 3 hrs. and filtered, the residue washed with hot EtOH, the combined alc. solns. evaporated, and the residue sublimed at 160-70°/15 mm. yield 52% 2-aminopyrazine-3-carboxylic acid anilide (XXIX), needles, m. 106-7° (EtOH). XXIX (2.0 g.) and 50 cc. 10% aqueous NaOH refluxed 2.5 hrs., diluted with 50 cc. H₂O, cooled, and extracted with Et₂O, and the aqueous layer adjusted to pH 5 gave 2-aminopyrazine-3-carboxylic acid (XXX), m. 200-1°; the Et₂O extract evaporated and the residual oil treated with Ac₂O gave 0.41 g. AcNHPh, m. 112-13°. XXII (3.75 g.), 40 g. Raney Ni, and 400 cc. EtOH refluxed 3 hrs. with stirring gave in the usual manner 0.24 g. unchanged XXII and 1.35 g. 2-PhCH₂NH analog (XXI) of XXVII, needles, m. 125-6° (EtOH). XXXI (1.0 g.) and 10 cc. 10% aqueous NaOH refluxed 2 hrs., adjusted to pH 4 with dilute HCl, cooled, and filtered gave 0.78 g. 2-PhCH₂NH derivative of XXX, plates, m. 166.5-68° (aqueous EtOH). XXVI (2 g.), 20 g. Raney Ni, and 200 cc. EtOH refluxed 4 hrs. with stirring gave 0.93 g. 5-Me derivative of XXVII, m. 203-4° (MeOH). XXV gave similarly 51.5% 6-Me derivative (XXXII) of XXVII, pale yellow, m. 235-6° (sublimed at 160-70°/18 mm.). XXXII (1.0 g.) and 10 cc. 10% aqueous NaOH refluxed 2 hrs., adjusted to pH 4 with dilute HCl, cooled to 0°, and filtered gave 0.72 g. 6-Me derivative of XXX, m. 211-12° (decomposition) (aqueous EtOH).

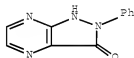
IT 109966-85-0P, 3H-Pyrazolo[3,4-b]pyrazin-3-one,
1,2-dihydro-5,6-dimethyl-2-phenyl- 118898-67-0P,
3H-Pyrazolo[3,4-b]pyrazin-3-one, 1,2-dihydro-2-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 109966-85-0 HCAPLUS

CN 3H-Pyrazolo[3,4-b]pyrazin-3-one, 1,2-dihydro-5,6-dimethyl-2-phenyl- (CA INDEX NAME)



RN 118898-07-0 HCAPLUS

CN 3H-Pyrazolo[3,4-b]pyrazin-3-one, 1,2-dihydro-2-phenyl- (6CI) (CA INDEX NAME)



L41 ANSWER 124 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1957:9344 HCAPLUS Full-text

DOCUMENT NUMBER: 51:9344

ORIGINAL REFERENCE NO.: 51:1949g-h

TITLE: The reaction of azobenzene and carbon monoxide

AUTHOR(S): Murahashi, Shunsuke; Horiie, Shigeki

CORPORATE SOURCE: Univ. Osaka

SOURCE: Journal of the American Chemical Society (1956), 78, 4816-17

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 51:9344

ED Entered STN: 22 Apr 2001

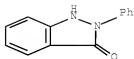
AB cf. C.A. 50, 10044g. Ph2N2 reacts with 1 mole CO (150 atmospheric pressure in all cases) at 190° in the presence of Co2(CO)8 to yield 55% 2-phenylindazoline (I), m. 204°, a small amount of 3-phenyl-2,4-dioxo-1,2,3,4-tetrahydroquinazoline (II), and (PhNH)2CO. Ph2N2 with 2 moles CO at 230° yielded 80% II, m. 277°. The yield was less when Fe(CO)5 was used instead of Co2(CO)8. p-ClC6H4N2Ph with CO and Co2(CO)8 at 230° yielded 23.8% 2-phenyl-5-chloroindazolone, m. 233°, and 45% 3-phenyl-6-chloro-2,4-dioxo-1,2,3,4-tetrahydroquinazoline, m. 264°; p-Me2NC6H4N2Ph yielded 80% 2-phenyl-5-dimethylaminoindazolone, m. 217°, and 18% 3-phenyl-6-dimethylamino-2,4-dioxo-1,2,3,4-tetrahydroquinazoline, m. 281°.

IT 17049-65-9F, 3-Indazolinone, 2-phenyl- 28561-70-8F, 3-Indazolinone, 5-chloro-2-phenyl- 101091-21-8F, 3-Indazolinone, 5-dimethylamino-2-phenyl-
RL: PREP (Preparation)

(preparation of)

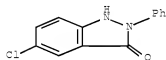
RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



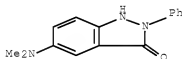
RN 28561-70-8 HCAPLUS

CN 3-Indazolinone, 5-chloro-2-phenyl- (6CI, 8CI) (CA INDEX NAME)



RN 101091-21-8 HCAPLUS

CN 3-Indazolinone, 5-dimethylamino-2-phenyl- (6CI) (CA INDEX NAME)



L41 ANSWER 125 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1954:18298 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 48:18298

ORIGINAL REFERENCE NO.: 48:3342h-i,3343a

TITLE: Isoxazole derivatives. V. Reaction of hydrazine on 5-aminoisoxazoles. 1

AUTHOR(S): Kano, Hideo

CORPORATE SOURCE: Shionogi & Co., Amagasaki

SOURCE: Yakugaku Zasshi (1953), 73, 383-7

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

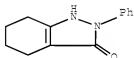
ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 47, 6936g. O.N:CR.CR':CNH₂ (I, R = Me) (IA) (5 g.) and 5 g. 50% N₂H₄.H₂O heated 2.5 hrs. on a water bath, and the product filtered and recrystd. from H₂O give 2.5 g. NH.NH.CO.CR':CR (II, R = Me) (IIA), prisms, m. 271-2°; 1 g. IIA and 2 ml. Ac₂O boiled 30 min., cooled, a small amount of water added, and the precipitate recrystd. from MeOH give NAc.NAc.CO.CR':CR (III, R = Me) (IIIA), needles, m. 54°. Similarly are prepared the following derivs. of I, II, and III, resp. (R, R', and m.p. given): Me, Et, 89-90°, 229-30°, 57°; Me, Pr, 77-8°, 211-2°, 40-1°; Me, PhCH₂, 79°, 230-1°, 69°; (R + R' =) (CH₂)₄, 119° 285-6° (decomposition), 79-80°. IA (5 g.) and 5 g. PhNNH₂ heated 8 hrs. at 100° and the product extracted with Et₂O give 1.9 g. 4,4'-bis(1-phenyl-3,4-dimethyl-5-pyrazolone), prisms, m. 165°. 3-Methyl-, 3-phenyl-, 3-benzyl-4-phenyl-, 3-ethyl-4-methyl-, and 3-butyl-4-propyl-5-aminoisoxazole

with N2H4.H2O or PhNHNH2 do not give pyrazolone derivs. AcCHMeCONH2 (0.5 g.) and 1 g. 50% N2H4.H2O heated 15 min. on a water bath and the product recrystd. from alc. give IIA, m. 270-1°.

IT 62221-94-7P, 3-Indazolinone, 4,5,6,7-tetrahydro-2-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 62221-94-7 HCAPLUS
 CN 3H-Indazol-3-one, 1,2,4,5,6,7-hexahydro-2-phenyl- (CA INDEX NAME)



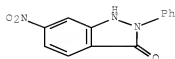
L41 ANSWER 126 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1934:44966 HCAPLUS Full-text
 DOCUMENT NUMBER: 28:44966
 ORIGINAL REFERENCE NO.: 28:5445c-f
 TITLE: Isomerization of 4,6-dinitrobenzylideneaniline
 AUTHOR(S): Secareanu, S.; Lupas, I.
 SOURCE: Bull. soc. chim. [5] (1934), 1, 373-80
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

ED Entered STN: 16 Dec 2001

AB cf. C. A. 28, 4047.9. The relations between an o-NO2 radical and the -CH=N- group as demonstrated by the isomerization of 2,4,6- (O2N)3C6H2CH:NPh (I) have been elucidated by a study of the analogous isomerization of the corresponding dinitro and o-nitro compds. A mixture of 3 g. of 2,4-(O2N)2C6H3CH:NPh, m. 133°, and 3 g. powdered Na2CO3 in 30 cc. EtOH was refluxed for 7 hrs. and filtered while hot. The cold solution was filtered and treated with AcOH, yielding 0.45 g. of crystalline 6-nitro-3-hydroxy-2-phenylindazole (II), C13H9N3O3, m. above 260°; Ac derivative, C15H11N3O4, m. 190-1°; Bz derivative, m. 171°. Concentration of the mother liquor and extraction with cold CHCl3 produced a Na salt, exploding on heating, which, on treatment with HCl, gave 6-nitro-1-N-hydroxy-2-phenylindazolone (III), C13H9N3O4, m. 166-7°. The addition of excess EtI to a suspension of 0.4 g. of the Ag salt of II in C6H6 yielded, on boiling for 30 mins., needle-shaped crystals of 6-nitro-1-N-hydroxy-3-ethoxy-2-phenylindazolone, C15H13N3O4, m. 64-5°. The formation of indazolone derivs. from I and II shows that this transformation is a characteristic property of these o-nitrobenzylideneanilines. Under the action of alc. Na2CO3 III is evidently susceptible of transformation into II. Prolonged treatment with alc. Na2CO3 leaves o-O2NC6H4CH:NPh unchanged.

IT 403665-52-1, 3-Indazolol, 6-nitro-2-phenyl-
 (and derivs.)
 RN 403665-52-1 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-6-nitro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 127 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1926:20421 HCAPLUS Full-text
 DOCUMENT NUMBER: 20:20421
 ORIGINAL REFERENCE NO.: 20:2495h-1,2496a-h
 TITLE: Miscellaneous observations on indazole derivatives
 AUTHOR(S): v. Auwers, K.; Strodtter, P.
 SOURCE: Berichte der Deutschen Chemischen Gesellschaft
 [Abteilung] B: Abhandlungen (1926), 59B,
 529-38
 CODEN: BDCBAD; ISSN: 0365-9488
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

ED Entered STN: 16 Dec 2001

AB 1. Arylhydroxyindazole and 3-arylindazoles. It had been found (cf. C. A. 16, 3654 and earlier papers) that the diazo compds. obtained from o-NH₂ ketones H₂CN₂C₆H₄COR give with Na₂SO₄ (the action of which may be strengthened by Na-Hg) 3-alkylindazoles when R is an alkyl, but when R is Ph the expected 3-phenylindazole (I) is formed only in subordinate amount, the chief product being 2-hydroxy-3-phenylindazole which is slowly converted by boiling alkalis into the 3,2-isomer. I is also noteworthy in that it occurs in 2 mutually interconvertible forms. The results described in the present paper indicate that the reaction with Na₂SO₃ proceeds essentially in the same way in all cases where R is an aryl residue; 4'-methyl- (II) and 4'-methoxy-2-aminobenzophenone (III) yield chiefly 3-p-tolyl- (IV) and 3-p-anisyl-2-hydroxyindazole (V), which, like the Ph derivative, are rather unstable compds. of acid character, lose N and change into MeC₆H₄COPh and MeOC₆H₄COPh, resp., when heated above their m. p., are rearranged by boiling alkalis into their 2,3-isomers and are reduced by SnCl₂ to 3-p-tolyl- (VI) and 3-p-anisylindazole (VII). Thus far, it has not been possible to isolate the VI and VII in 2 different forms, but as the products obtained showed no sharp m. p. after repeated crystns. and other purifications the possibility of the existence of 2 such forms is not excluded; not enough of them was available for a more thorough study of their properties. 2. Reductive cleavage of 2-phenylindazole. According to Paal, 2-phenylindazole (VIII) in hot absolute alc. with Na gives its 1,3-dihydro derivative (IX), m. 98°. In attempting to repeat his work, v. A. and S. obtained, instead of IX, o-H₂CN₂C₆H₄CH₂NHPh (X), m. 87°; the experiment was then repeated 5 times with slight modifications in the conditions and in 3 cases X was again obtained while in the other 2 the product had the same appearance and slight solubility in alc. as IX but m. 153° (in a later preparation the m. p. could not be raised above 136°); analysis indicated that these preps. were not quite pure IX; on short heating on the H₂O bath they regenerated VIII and also changed rapidly in the air. It seems clear that the primary product of reduction is IX but that on more energetic treatment with Na and alc. the pyrazole ring is ruptured with surprising ease. 3. Some derivatives of indazole-3-carboxylic acid. Most esters of indazole-1-carboxylic acid when heated under suitable conditions lose CO₂ with formation, together with resinous products, of both 1- and 2-alkylindazoles, the latter sometimes, indeed, being the chief products. To determine whether a negative substituent in position 3 would influence the course of this reaction the decomposition of some indazole-1,3-dicarboxylic esters has been studied. These compds. are readily obtained when, e. g., Me indazole-3-carboxylate (XI) is boiled with ClCO₂Me or ClCO₂Et and on decomposition they yield, together with products of more deep-seated decomposition, the 1-alkyl derivs. exclusively; apparently the 3-CO₂Me group hinders the migration of the alkyl group to the adjacent 2-N atom. Similarly, while indazole heated with allyl bromide gives exclusively the 2-derivative and I gives both the 1- and 2-derivs., Et indazole-3-carboxylate (XII) gives

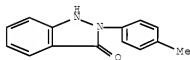
only the 1-derivative With o-O2NC6H4COCl, which is especially well adapted to the preparation of 2-acylindazoles, XII gives no 2-derivative IV (yield, 65%), colorless or only faintly yellowish and almost odorless, stable for a long time, but not indefinitely in cork-stoppered vessels but quickly decomp. in the air and light, m. 119° (gas evolution). 2,3-Isomer (obtained in about 50% yield, together with about 1 g. p-MeC6H4COPh, m. 59°, b. 327-8°, from 3 g. IV in 2% NaOH treated with steam until no more oil distilled over (about 2.5 hrs.)), begins to turn brown 190°, shrinks 200° and m. 215°, soluble in concentrated H2SO4 with yellow color; acetate, m. 98°; benzoate, m. 154-5°. VI, softens 91°, m. 97-8°; picrate, yellow, m. 147-8°; Ac derivative, m. 79.5-80.5°. V, m. 132° (gas evolution), is partly changed on attempted recrystn. from C6H6; 2,3-isomer (2.6 g., together with 0.3 g. p-MeOC6H4COPh from 4 g. V), darkens 153°, sinters 163°, gives an intensely yellow color in alc. with Ca(OC1)2, soluble in concentrated H2SO4 with orange-yellow color; acetate, m. 110°; benzoate, m. 139.5-40°. VII, oil which on distillation (about 205°) under 10 mm. changed into a resinous mass and was obtained in crystalline form, m. 110-1°, only after purification through the Ac derivative, m. 105-6°; picrate, yellow, m. 147-8°. Contrary to an earlier statement VIII does form, in very concentrated alc. or Et2O solution, Freundler's picrate, yellow, m. 93-4°. Di-Me indazole-1,3-dicarboxylate (yield, almost quant.), m. 174-5° (gas evolution), regenerates XI with aqueous KOH in cold Me2CO; distilled at 150-80° under 12 mm. it yields the 1-Me derivative, m. 77-8°, of XI. 1-Et 3-Me ester, faintly yellowish, m. 116°, b13, 218° without decomposition but under atmospheric pressure it yields the 1-Et derivative of XI. 1-Allylindazole-3-carboxylic acid, from XI and allyl bromide heated at 120-30° in sealed tubes and subsequently saponified m. 147°. Et 1-o-nitrobenzoylindazole-3-carboxylate, m. 182-3°, is not attacked by HCl in dry Et2O; attempts to prepare an isomer by treating the Ag salt of XII with O2NC6H4COCl gave a substance m. 132.5-3.5°.

IT 74152-86-8, 3-Indazolol, 2-p-tolyl- 74152-89-9,
3-Indazolol, 2-p-anisyl-

(and derivs.)

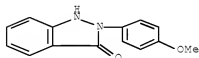
RN 74152-88-8 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-methylphenyl)- (CA INDEX NAME)



RN 74152-89-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-(4-methoxyphenyl)- (CA INDEX NAME)



DOCUMENT NUMBER: 18:1709
 ORIGINAL REFERENCE NO.: 18:263a-i
 TITLE: New cases of isomerism. II. Structural association
 AUTHOR(S): Heller, Gustav; Kohler, Willi
 SOURCE: Berichte der Deutschen Chemischen Gesellschaft
 [Abteilung] B: Abhandlungen (1923), 56B,
 1595-600

CODEN: BDCBAD; ISSN: 0365-9488

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

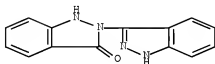
ED Entered STN: 16 Dec 2001

GI For diagram(s), see printed CA Issue.

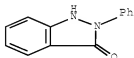
AB cf. C. A. 11, 2778. It was shown in the earlier paper that an unexpected isomerism exists in p-lactams between the forms containing the grouping -NH.C6H4.CO- and those with the grouping -N : C6H4: C(OH)-. This was proved with the 3 pairs of isomers γ -ketohydroquinaldine (I) and γ -hydroxyquinaldine (II) (and the corresponding CO2H acids), 3-keto-2-phenyl-1,3-dihydroindazole (III) and 3-hydroxy-2-phenylindazole (IV), and isatin (V) and isatole (VI). Thode (J. prakt. Chemical 69, 92(1904)) by heating o-H2NC6H4CONHNH2 at 200° obtained a compound to which he assigned the 3-keto-1, 3-dihydroindazole structure (VII) of Fischer's o-hydrazinobenzoic anhydride, while to F.'s compound he gives the structure VIII. H. and Jacobsohn have shown, however, that F.'s compound has the structure VII (C. A. 15, 3480), and it seemed quite probable that F.'s and T.'s compds. are isomers of the type mentioned above, T.'s product being 3-hydroxyindazole (IX). While VII yields a di-Ac derivative, IX on cautious acetylation gives a 2-mono-Ac derivative (X) which is converted by hot AcOH into the ether XI and this with boiling HCl loses only one Ac group. With HNO2 IX does not give the expected alkali-soluble mono-NO derivative but an alkali-insol. bimol. di-NO derivative (XII), whose formation may be explained by assuming that the NO group first attaches itself to the 2-N atom of IX and that the product rearranges into the 2-N derivative of VII which then reacts further with the HNO2 to give XII. With P chlorides IX yields a Cl-free bimol. compound (XIII) whose composition corresponds to 2IX - H2O but whose di-Ac derivative differs from XI; XIII must therefore have a different structure, most likely XIV. Just as VI is trimol. in solvents, so also are IX and II in camphor (II in boiling Me2CO likewise). However, there is a gradual difference in this association; while VI is trimol. in PhOH, IX is predominantly bimol. (which may also be considered as incipient solvate formation) and II is monomol, and even in camphor in the more dilute solns. shows beginning dissociation. This tendency of the p-lactams to form trimers explains the fact that both tautomeric forms can exist simultaneously; it seems that in these cases there is a new kind of association, which may be designated as structural association, as the result of which a form, in and of itself tautomeric, is stabilized. Certain solvents can in individual cases break up the polymer without rearrangement, forming solvates, and there likewise exist derivs. with a simple mol. weight which again may be associated. IX (benzoylisoprazolone), obtained in 0.3-0.4 g. yield from 2 g. o-H2NC6H4CONHNH2 heated 4-5 hrs. at 200-10° with 1 g. quinoline, forms leafy crystals with a faint brown tinge, m. 206°, easily soluble in dilute NaOH, gives in alc. with FeCl3 a dirty blue color, mol. weight in PhOH 296, in camphor 382-421. Mol. weight of II in camphor 328-468, in PhOH 185, in Me2CO 512; of VI in camphor 441. X (0.7 g. from 0.7 g. IX shaken with 4 cc. Ac2O), m. 188° (foaming), soluble in dilute NaOH, gives no color with FeCl3 in alc., mol. weight in PhOH 175. Bis-N-acetylindazyl 3-ether (XI) (7.3 g. from 0.5 g. X boiled 0.5 hr. in AcOH), m. 190°, easily soluble in concentrated HCl, insol. in alkali, mol. weight in camphor 340, converted by heating 2 hrs. on the H2O bath with concentrated HCl into a mono-Ac derivative, m. 206°, easily soluble in alkalies and acids, gives a precipitate with NaNO2 in HCl, mol. weight in camphor 300. Bisbenzoylisoprazolyl (XIII), from 0.5 g. IX boiled 5 min. with 7 cc. POC13 and 0.5 PC15, m. 228°, soluble in AcOEt, alc. and ligroin with

bluish red fluorescence, mol. weight in camphor 258, gives with hot Ac2O a compound m. 250°. 1,2-Dinitroso-3-ketodihydroindazole (XII), faintly yellow, m. 249° (decomposition), mol. weight in camphor 440, does not give the Liebermann reaction.

IT 861360-69-2P, 3(1)-Indazolone, 2-(3-indazolyl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 861360-69-2 HCAPLUS
 CN 3(1)-Indazolone, 2-(3-indazolyl)- (2CI) (CA INDEX NAME)



L41 ANSWER 129 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1923:5527 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 17:5527
 ORIGINAL REFERENCE NO.: 17:1020g-h
 TITLE: 3-Hydroxy-2-phenylindazole
 AUTHOR(S): Heller, Gustav
 SOURCE: Berichte der Deutschen Chemischen Gesellschaft
 [Abteilung] B: Abhandlungen (1922), 55B,
 2680
 CODEN: BDCBAD; ISSN: 0365-9488
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 ED Entered STN: 16 Dec 2001
 AB H. does not agree with v. Auwers and Huttenes (C. A. 16, 3654) that
 Freundler's 3-hydroxy-2-phenylindazole, m. 214°, which dissolves in alkali
 with a bright yellow color, and H.'s isomer, m. 204°, soluble in alkali almost
 without color (C. A. 11, 2778), are the same substance in different degrees of
 purity.
 IT 17049-65-9P, 3-Indazolol, 2-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 17049-65-9 HCAPLUS
 CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 130 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1923:5526 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 17:5526
 ORIGINAL REFERENCE NO.: 17:1019i,1020a-g

TITLE: The diazo reaction in the carbazole series.
 AUTHOR(S): Carbazole-3-diazoimine and -3-diazonium salts
 Morgan, G. T.; Read, H. N.
 SOURCE: Journal of the Chemical Society, Transactions (1922), 121, 2709-17
 CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

ED Entered STN: 16 Dec 2001

GI For diagram(s), see printed CA Issue.

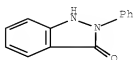
AB The outstanding features in regard to carbazole-3-diazonium salts are their stability compared with the corresponding diazo derivs. of C₆H₆, Ph₂ and C₁₀H₈ series and their pronounced yellow color. Carbazole-3-diazonium chloride (I) was prepared by adding 20% aqueous NaNO₂ to a thin paste of the 3-NH₂.HCl derivs. in dilute HCl at 8°; crystallized from H₂O it forms fan-shaped clusters of yellow needles with 2 mols. H₂O, which became green at 98° and decomposed 102°. The anhydrous salt darkened at 106-10° and decomposed explosively at 153°. The chloroaurate, bright yellow, sparingly soluble compound, is quite stable in the dark but darkened on exposure to light. Treated with NH₄OH in H₂O I gives carbazole-3-diazoimine (II), bright orange-red needles which, heated rapidly, exploded at 95°, but heated slowly, darkened between 80-105° and did not m. 300°. It decomps. almost at once in the sunlight and explodes on rubbing or by percussion or when placed near a flame. It is decomposed by H₂O, forming an ill defined product which does not m. 300°. HCl regenerated I. I or II, treated with β-C₁₀H₇OH, gave carbazole-3-azo-β-naphthol, reddish violet needles, m. 279° (decomposition); with resorcinol, carbazole-3- azoresorcinol, violet, m. 265-70°. Carbazole-3-azo-β- naphthylamine, reddish brown needles, m. 260-3°. Carbazole-3-diazocyanide, NH:C₁₂H₇N₂CN, by the action of KCN upon I in acid or alkaline solution, small, brick-red needles, decompose 155-60°. The slow rate of condensation with β-C₁₀H₇OH suggested the anti-form. Carbazole-3-diazonium nitropruside, amorphous light yellow precipitate which becomes green at 150° and decomps. explosively at 160°. 3-Triazacarbazole (carbazole-3-azoimide) (III), by the action of NaN₃, lustrous plates, m. 176-7° (decomposition). It becomes brown on exposure to light and decomps. with considerable violence when dropped into H₂SO₄. Ethyl carbazole-3-azoacetoacetate, golden yellow prismatic needles, m. 193°. N-Ethylcarbazole-3-diazonium chloride, golden yellow needles with 2H₂O, m. 149-50° (decomposition). It is not very sensitive to the action of light. The chloroaurate is a bright yellow compound. The dichromate forms bright yellow acicular prisms and is comparatively stable.. The cyanide forms bright red needles and decomps. 148-55°. The nitroprusside seps. as bright yellow microneedles. Ethyl N-ethylcarbazole 3-azoacetoacetate, golden yellow needles, m. 125°. The action of NH₄OH on the chloride gave a light brown microcryst. product, charring at 150-5°, which is probably an external diazo-oxide. Concentrated HCl gave a greenish blue indefinite product and the chloride.

IT 17949-65-9P, 3-Indazolol, 2-phenyl-
 RL: PREP (Preparation)

(preparation of)

RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



L41 ANSWER 131 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1921:16476 HCAPLUS Full-text

DOCUMENT NUMBER: 15:16476

ORIGINAL REFERENCE NO.: 15:3082i,3083a-f

TITLE: Influence of nitro groups on the reactivity of substituents in the benzene nucleus. IV. The condensation of ethyl 3- and 5-nitro-2-chlorobenzoates with hydrazines

AUTHOR(S): Kenner, James; Witham, Ernest

CORPORATE SOURCE: Univ. Sheffield

SOURCE: Journal of the Chemical Society, Transactions (1921), 119, 1053-8

CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 15:16476

ED Entered STN: 16 Dec 2001

GI For diagram(s), see printed CA Issue.

AB N2H4.H2O and 2,5-Cl(O2N)C6H3CO2Et gave a mixture of 4-nitrocarbethoxyphenylhydrazine, C9H11O4N3, yellow needles, m. 172° (acetate, C11H18O4N3, faintly green needles, m. 191.5°; benzaldehyde derivative, C16H15O4N3, prismatic needles, m. 165-6°), and 5-nitro-3-keto-1,3-dihydroindazole, C7H5O3N3 (A) by acidification of the filtrate, small reddish brown aggregates of prisms, m. 273° (decomposition); acetate, C9H7O4N3 small, faintly yellow prisms, m. 239°; sodium salt, dark orange-red powder; reduced with Sn and HCl, the hydrochloride of the 5-amine derivative C7H7ON3.2HCl, was obtained as needles, m. 286° (decomposition), which become slate color on keeping. The action of PhNHNH2 on 2,5-Cl(O2N)C6H3CO2Et gave 4-nitro-2-carbethoxyhydrazobenzene (B), C15H15O4N3, yellow prisms, m. 133°, which on oxidation with HgO gave 4-nitro-2-carbethoxyazobenzene, red, hexagonal plates, m. 70-1°. Boiling B with 0.5 N NaOH for 20 min. gave 5-nitro-3-keto-2-phenyl-1,3-dihydroindazole, O2NC6H3.NH.NPh.CO (C), faintly green needles, m. 270-3°. Sodium salt, dark brownish red crystalline precipitate 3-Chloro-5-nitroindazole, (I) was prepared by heating A with POCl3 5 hrs. at 120-30°; it forms faintly yellow needles, m. 210-1°. 3-Chloro-5-nitro-2-phenylindazole, C13H8O2N3Cl, as above from C, small prisms, m. 165°. 7-Nitro-3-keto-1,3-dihydroindazole (II). by the action of N2H4.H2O on 2,3-Cl(O2N)C6H3CO2Et, Cu-colored plates from glacial AcOH, m. 290°. Acetate, brown needles, m. 196-7°. Sodium salt, PhNHNH2 gave 2-nitro-6-carbethoxyhydrazobenzene, C15H15O4N3, greenish yellow needles, m. 119°, which are not oxidized by HgO. 7-Nitro-3-keto-2-phenyl-1,3-dihydroindazole, C13H9O3N3, minute greenish yellow prisms, m. 185°. Sodium salt, gives a purple solution and has a tendency to sublime at 140°.

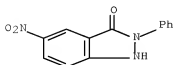
IT 861360-67-6P, 3(1)-Indazolone, 5-nitro-2-phenyl-

RL: PREP (Preparation)

(preparation of)

RN 861360-67-0 HCAPLUS

CN 3(1)-Indazolone, 5-nitro-2-phenyl- (2CI) (CA INDEX NAME)



L41 ANSWER 132 OF 132 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1917:13748 HCAPLUS Full-text

DOCUMENT NUMBER: 11:13748

ORIGINAL REFERENCE NO.: 11:2778i,2779a-f

TITLE: New cases of isomerism

AUTHOR(S): Heller, Gustav

SOURCE: Berichte der Deutschen Chemischen Gesellschaft (1916), 49, 2757-74

CODEN: BDCGAS; ISSN: 0365-9496

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 11:13748

ED Entered STN: 16 Dec 2001

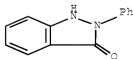
AB through J. Chemical Society 112, I, 219-20; cf. C. A. 11, 937. Desmotropism seems to be exhibited by 3-hydroxy-2-phenylindazole. On heating o-PhNNHC6H4CO2H with Ac2O a stable form (I) seps. in needles or rods, m. 204°, whose benzoate, long spikes, m. 180.5°, but solution in POC18 converts it into the labile ketonic form (II) (Freundler, Compt. rend. 143, 909(1906)), which is again transformed into the enol form by successive crystns. In addition to the lactam, and lactim forms of isatin, known in the Me derivs. (III) and (IV), the remaining alternative (V), designated "isatol," has now been isolated by shaking isatin in hot alc. with AgOAc; the N-silver salt seps. at once as a grayish red powder soluble in C5H5N with deep bluish red color. The salt is warmed with BzCl and C6H6, the AgCl removed and the filtrate allowed to stand, whereupon (V) seps. and crysts. from methylal in red prisms, m. 194.5°, insol. in Na2CO3 and NH4OH, soluble in NaOH with orange-red color which becomes pale on heating, and acids precipitate ordinary isatin. Ac2O, BzCl, PhNNH2, NaHSO3, MeI and NaNO2 have no action on (V) but CH2N2 gives the methyl ether, pale yellow amorphous substance. That the H atom in the 3 forms is most acidic in the imino compound is shown by the fact that isatin is soluble in NH4OH whereas (V) is not; isatin decomps. AgOAc and the α -oxime is soluble in NaOH with deep blue color while the Et ether of the β -oxime is only phenolic and forms a yellow solution α -Isatoxime, C6H4.CO.C(:NOH).NH, is conveniently prepared from NH2OH and (IV) and on warming with NaOH changes into C6H4.CO.NH.CONH. The various salts of isatin and its ethers and oximes owe their differences in color mainly to the different attachments of the metal, the N-salts being usually deeper in color than the O-salts.

IT 17049-65-9, 3-Indazolol, 2-phenyl-

(desmotropism of, and benzoate)

RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



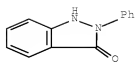
IT 17049-65-9P, 3(1)-Indazolone, 2-phenyl-

RL: PREP (Preparation)

(preparation of)

RN 17049-65-9 HCAPLUS

CN 3H-Indazol-3-one, 1,2-dihydro-2-phenyl- (CA INDEX NAME)



Search History

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L2          22 SEA ABB=ON  PLU=ON  (112253-72-2/BI OR 112677-17-5/BI OR
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          OR 455-14-1/BI OR 5720-06-9/BI OR 65753-47-1/BI OR 852620-72-5
          /BI OR 852620-74-7/BI OR 852620-76-9/BI OR 852620-77-0/BI OR
          852620-78-1/BI OR 852620-79-2/BI OR 852620-80-5/BI OR 852620-81
          -6/BI OR 852620-82-7/BI OR 852620-83-8/BI OR 852620-84-9/BI OR
          852620-85-0/BI OR 852620-86-1/BI)
L3          STRUCTURE UPLOADED
L4          17 SEA SSS SAM L3
L5          STRUCTURE UPLOADED
L6          18 SEA SSS SAM L5
L7          0 SEA ABB=ON  PLU=ON  L6 AND L2
L8          265 SEA SSS FUL L5
L9          0 SEA ABB=ON  PLU=ON  L8 AND L2

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L11         50 SEA SSS SAM L10
L12         0 SEA ABB=ON  PLU=ON  L11 AND L2

FILE 'REGISTRY' ENTERED AT 10:43:37 ON 04 MAR 2008
L13         STRUCTURE UPLOADED
L14         36 SEA SSS SAM L13
L15         0 SEA ABB=ON  PLU=ON  L14 AND L2
L16         660 SEA SSS FUL L13
L17         8 SEA ABB=ON  PLU=ON  L16 AND L2

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L19         268 SEA ABB=ON  PLU=ON  L18 AND (PRY<=2003 OR AY<=2003 OR PY<=2003)

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L20         4726004 SEA ABB=ON  PLU=ON  5-6/SZ
L21         10 SEA ABB=ON  PLU=ON  L20 AND L2
L22         STRUCTURE UPLOADED
L23         24 SEA SUB=L16 SSS SAM L22
L24         436 SEA SUB=L16 SSS FUL L22
L25         6 SEA ABB=ON  PLU=ON  L24 AND L2
L26         2 SEA ABB=ON  PLU=ON  L17 NOT L25

FILE 'HCAPLUS' ENTERED AT 11:02:11 ON 04 MAR 2008
L27         245 SEA ABB=ON  PLU=ON  L24

FILE 'REGISTRY' ENTERED AT 11:26:53 ON 04 MAR 2008
L28         STRUCTURE UPLOADED
L29         22 SEA SUB=L16 SSS SAM L28

FILE 'REGISTRY' ENTERED AT 11:36:16 ON 04 MAR 2008
L30         22 SEA SUB=L16 SSS SAM L28

FILE 'REGISTRY' ENTERED AT 14:15:52 ON 04 MAR 2008
L31         STRUCTURE UPLOADED

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Serial No.:10/579,355

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 L33 0 SEA ABB=ON PLU=ON L32 AND L2
 L34 248 SEA SUB=L16 SSS FUL L31
 L35 6 SEA ABB=ON PLU=ON L34 AND L2

FILE 'HCAPLUS' ENTERED AT 14:26:04 ON 04 MAR 2008
 L36 144 SEA ABB=ON PLU=ON L34

FILE 'HCAPLUS' ENTERED AT 14:28:45 ON 04 MAR 2008
 L37 133 SEA ABB=ON PLU=ON L36 AND (PRY<=2003 OR AY<=2003 OR PY<=2003)
 L38 24 SEA ABB=ON PLU=ON BURKAMP F?/AU
 L39 405 SEA ABB=ON PLU=ON FLETCHER S?/AU
 L40 1 SEA ABB=ON PLU=ON (L38 OR L39) AND L37

FILE 'HCAPLUS' ENTERED AT 14:32:59 ON 04 MAR 2008
 L41 132 SEA ABB=ON PLU=ON L37 NOT L40